

# An Introduction to Plasma and Feature Scale Modeling in the Semiconductor Industry

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## **Agenda**

- Plasmas in the Semiconductor Industry
- Plasma and Feature Scale Modeling
- Modeling Examples
  - ▶ Global models
  - ▶ Plasma uniformity
  - ▶ Plasma breakdown
  - ► Feature scale modeling
  - ▶ Plasma surface interaction
- Conclusions



## **Plasmas and the Semiconductor Industry**

- It's hard to picture life in 2025 without microelectronics—they're everywhere!
- Low-temperature plasmas are a key technology used for microelectronics manufacturing:
  - Etching
  - Deposition
  - Cleaning and surface preparation
  - Material modification



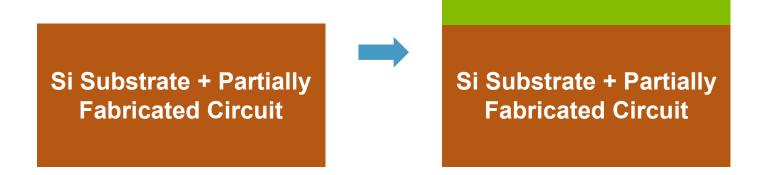




## **Plasmas and Microelectronics Fabrication**

Microelectronics fabrication requires 100s of processing steps, many plasma based.

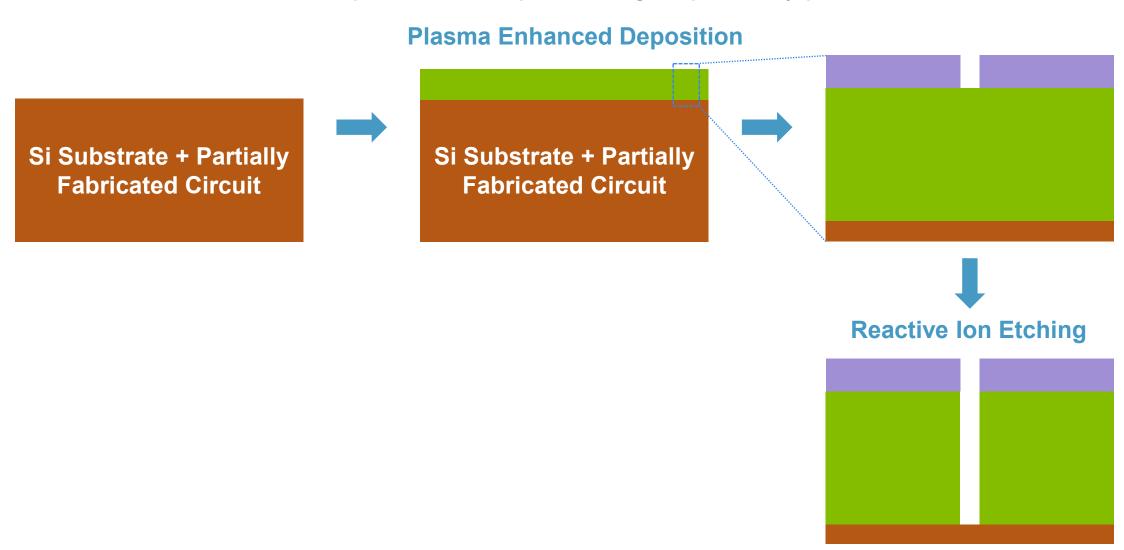
#### **Plasma Enhanced Deposition**





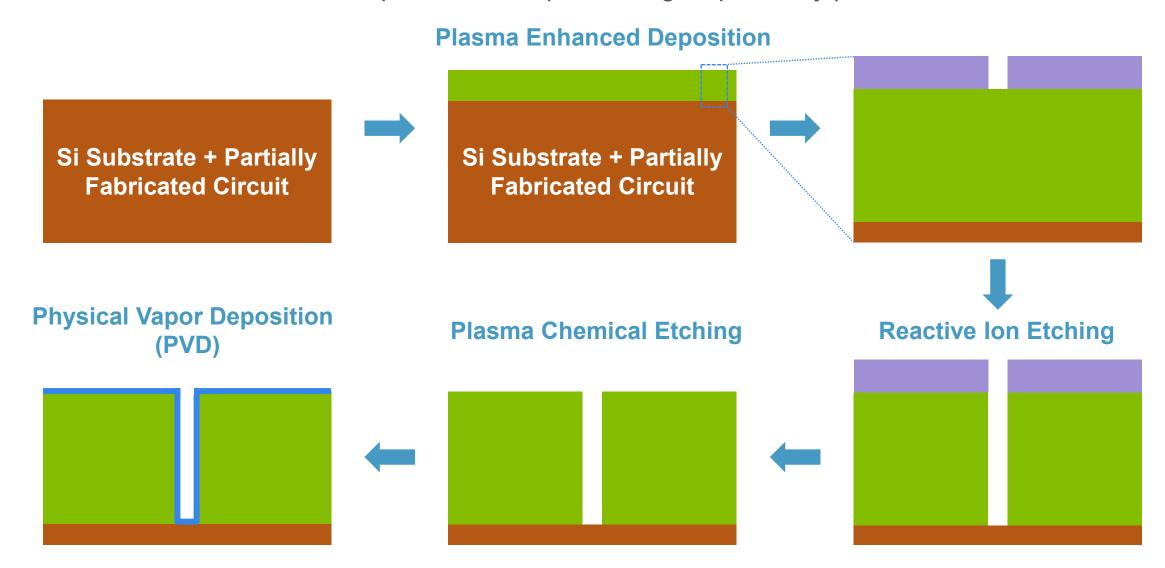
## **Plasmas and Microelectronics Fabrication**

Microelectronics fabrication requires 100s of processing steps, many plasma based.



#### Plasmas and Microelectronics Fabrication

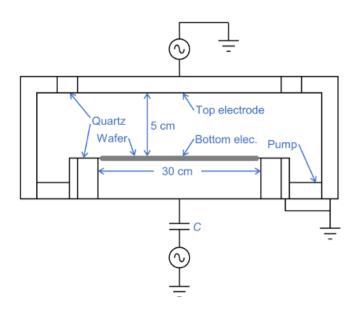
Microelectronics fabrication requires 100s of processing steps, many plasma based.



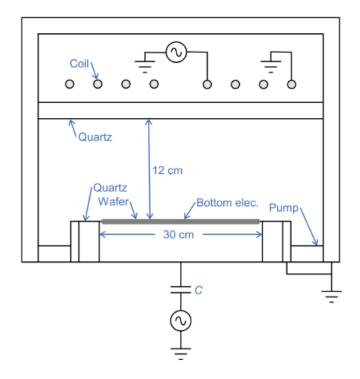
## **Typical Plasma Sources in Semiconductor Industry**

• Many plasma sources are used in the semiconductor industry including the following:

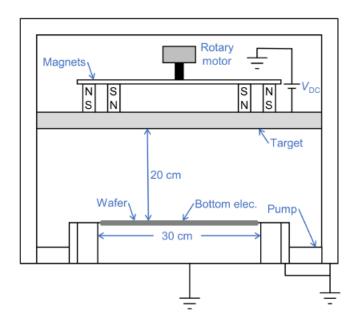
#### **Capacitively Coupled Plasma**



#### **Inductively Coupled Plasma**



#### **Magnetron Based PVD Source**



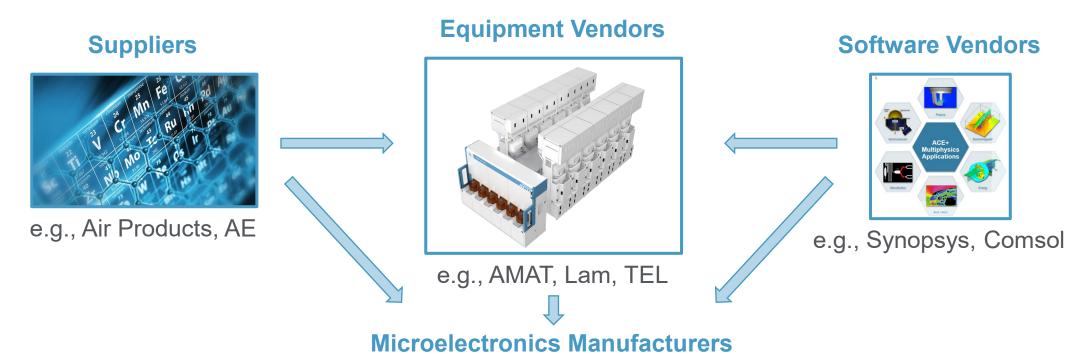
Rauf et al., J. Micro/Nanopattern. Mater. Metrol. 22, 041503 (2023)

Plasma and Feature Scale Modeling



## Plasma and Feature Scale Modeling Ecosystem in Semiconductor Industry

Semiconductor industry is one of the largest employers of plasma modeling engineers.





e.g., TSMC, Sony, Intel



## Plasma and Feature Scale Modeling Toolbox

- Plasma modeling engineers in industry:
  - ▶ Actively participate in R&D, product design, and customer communication
  - ▶ Work on a diverse set of technically challenging problems
  - Need strong foundation in plasma physics and plasma surface interactions to be successful



## Plasma and Feature Scale Modeling Toolbox

- Plasma modeling engineers in industry:
  - ▶ Actively participate in R&D, product design, and customer communication
  - Work on a diverse set of technically challenging problems
  - Need strong foundation in plasma physics and plasma surface interactions to be successful
  - Use a variety of specialized software tools

#### **Plasma Modeling**

- Global
- Fluid and hybrid
- Kinetic

#### **Feature Scale Modeling**

- String and level-set
- Monte Carlo

#### **Atomistic Modeling**

- Molecular dynamics
- Quantum chemistry

#### **General Tools**

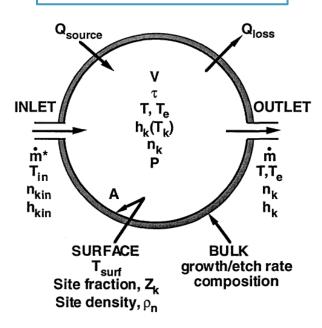
- Python
- Excel
- Fortran / C++

Rauf *et al.*, J. Micro/Nanopattern. Mater. Metrol. 22, 041503 (2023) Kuboi, J. Micro/Nanopattern. Mater. Metrol. 22, 041502 (2023) Alves *et al.*, Plasma Sources Sci. Technol. 27, 023002 (2018)

## Plasma Modeling – Global Models

- Global or 0D models use judicious assumptions to develop simple models for plasma systems:
  - ▶ Spatial shape of plasma,  $g_i(\mathbf{x})$
  - Power deposition mechanism
  - ▶ Electron energy distribution function (EEDF) or Boltzmann equation
- Global models are fast and can afford to model detailed chemistries.
- Plasma physics and chemistry expertise is critical to develop good global models.
- Available global models include:
  - Quantemol Global Model (<u>Quantemol-DB</u>)
  - ▶ ZDPlasKin

#### **Well-Stirred Reactor**



Lieberman and Lichtenberg, Principles of Plasma Discharges and Materials Processing (2025) Chabert and Braithwaite, Physics of Radio-Frequency Plasmas (2011) Meeks et al., AURORA, Sand-96-8218 (1996)

## Plasma Modeling – Fluid and Hybrid Models

- Fluid plasma models are the most widely used in industry.
- Fluid models are relatively fast, available in 1, 2, and 3-D, most mature and well-studied, and flexible with many physics options.
- Hybrid models add kinetic treatment of athermal electrons and ions in fluid models.
- Available fluid and hybrid plasma models include:
  - Quantemol-VT (HPEM)
  - ▶ CFD-ACE+ (ACE+ Applied Materials)
  - **COMSOL Plasma Module**
  - Vizglow (OverViz Lam Research)

Powered electrode Confinement grid  $P_{e} (10^{5} \text{ W/m}^{3})$ 

SiO<sub>2</sub> Top electrode

Fig. 1. (a) Electron density in the CCP reactor with the confinement grid, (b) another view of electron density in the reactor with confinement grid, (c) electron density in the system without the confinement grid, (d) electron power deposition without the confinement grid, and (e) electron power deposition in the reactor with confinement grid. Simulations are for 100 mtorr gas pressure in Ar, 500 W applied from bottom electrode at 60 MHz, and 7.5 cm interelectrode spacing. Only a 40° site is shown for clarity.

Kenney, Rauf, and Collins, IEEE Trans. Plasma Sci. 36, 1364 (2008)

Rauf et al., J. Micro/Nanopattern. Mater. Metrol. 22, 041503 (2023) Kushner, J. Phys. D: Appl. Phys. 42, 194013 (2009)

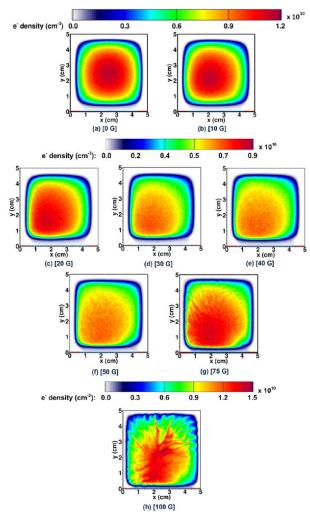
Alves et al., Plasma Sources Sci. Technol. 27, 023002 (2018)

## Plasma Modeling – Kinetic Modeling

- Kinetic plasma models become essential for simulating:
  - low pressure and magnetized plasmas
  - discharges where kinetic phenomena are important
- Particle-in-Cell with Monte Carlo Collisions (PIC/MCC) is the most widely used kinetic plasma modeling technique.
- PIC simulations are usually slow, and PIC codes are often physics-focused with limited bells-and-whistles for industrial use.
- Available PIC modeling codes include
  - EDIPIC (Princeton Plasma Physics Lab)
  - WarpX (Lawrence Berkeley Lab)
  - VSimPlasma (Tech-X)

Birdsall and Langdon, Plasma Physics via Computer Simulation, 1991

#### **Effect of Magnetic Field on Electron Density**



Ganta et al., Phys. Plasmas 31, 102107 (2024)



## Feature Scale Modeling – Monte Carlo

- Monte Carlo methods are commonly used to model plasma interaction with surfaces.
- These models approximate the material as a 2 or 3-D array of voxels representing atomic clusters.
- Plasma species with given fluxes and energy + angular distributions are introduced from the top.
- The reaction mechanism dictates the interaction of ions and neutrals from the plasma with the surface.
- Available Monte Carlo feature scale model include:

Kuboi, J. Micro/Nanopattern. Mater. Metrol. 22, 041502 (2023)

- MCFPM (University of Michigan)
- ▶ Pagasus FPSM2D

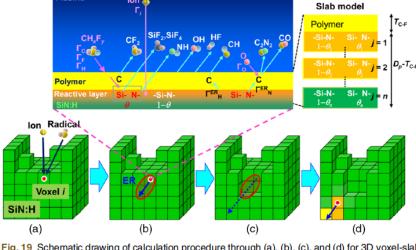


Fig. 19 Schematic drawing of calculation procedure through (a), (b), (c), and (d) for 3D voxel-slab model.69

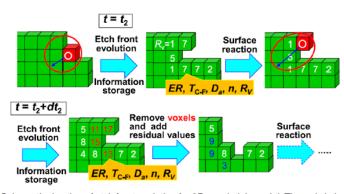
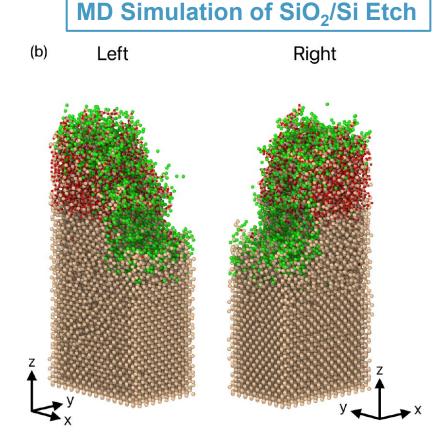


Fig. 20 Schematic drawing of etch front evolution for 3D voxel-slab model. The red circle at the red voxel represents an etched region related to the derive ER and red values in voxels exceed the threshold to be removed.65

## **Atomistic Modeling – Molecular Dynamics**

- Molecular dynamics (MD) is a widely used technique in material science and quantum chemistry.
- MD combines potentials (derived from ab-initio computations) with classical physics to simulate the dynamics of large cluster of atoms.
- MD is used by the low-temperature plasma community to study plasma etch processes.
- Availability and accuracy of potentials are important issues in MD modeling.
- Many MD models are available (MD Software Wikipedia) including:
  - ► <u>LAMMPS</u> (Sandia National Lab)



Mauchamp and Hamaguchi, J. Vac. Sci. Technol. A 40, 053004 (2022)

References

Frenkel and Smit, Understanding Molecular Simulation (2001)
Griebel, Knapek, and Zumbusch, Numerical Simulation in Molecular Dynamics (2010)
Mubin and Li, Extending and Modifying LAMMPS (2021)



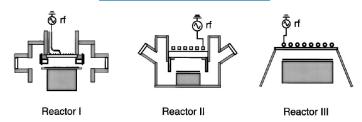
# Modeling Examples



## Ho – SiO<sub>2</sub> Etch in C<sub>2</sub>F<sub>6</sub> Plasma – Model

- Ho et al. developed a 0D model for SiO<sub>2</sub> etch in C<sub>2</sub>F<sub>6</sub> plasma using Aurora.
- C<sub>2</sub>F<sub>6</sub> mechanism: 28 species and 132 reactions.
- SiO<sub>2</sub> etch mechanism: 6 species and 85 reactions.
- Assumptions: spatially uniform, Maxwellian electrons.
- Tested the model using experimental data from 3 ICP reactors.

## **ICP Reactors**



## **Mechanism – C<sub>2</sub>F<sub>6</sub> Plasma and SiO<sub>2</sub> Etch**

saction No.	Reaction	A	В	C	ε	Notes	Reference
	Electron impact reaction						
(1)	$e^- + C_2F_6 \rightarrow C_2F_6 + e^-$	2.128E-7	-0.3252	3.676E3	0.14	V5 <sup>b</sup>	42
(2)	$e^- + C_2F_6 \rightarrow C_2F_6 + e^-$	6.788E-8	-0.4328	6.072E3	0.09	V6 <sup>b</sup>	42
(3)	$e^- + C_2F_4 \rightarrow C_2F_6 + e^-$	3.797E-4	-0.7779	2.192E4	0.15	V7*	42
(4)	$e^- + C_2F_4 \rightarrow C_2F_4 + e^-$	3.830E-3	-1.142	1.154E5	7.2	Ee.	42
(5)	$e^- + C_2F_4 \rightarrow C_2F_6 + e^-$	1.898E-12	0.6096	1.316E5	11.1	E <sup>c</sup>	42
(6)	$\sigma^- + C_2F_4 \rightarrow 2CF_3 + \sigma^-$	3.124E-8	0.1003	1.591E5	12.3	d	42
(7)	$e^- + C_2F_4 \rightarrow CF_1^+ + CF_1 + 2e^-$	2.483E-12	0.8790	1.637E5	15.5	•	43
(8)	$e^{-} + C_{2}F_{4} \rightarrow CF_{2}^{+} + CF_{4} + 2e^{-}$	3.297E-13	0.8655	2.408E5	17.3	e	43
(9)	$\sigma^- + C_2F_4 \rightarrow CF^+ + CF_4 + F + 2\sigma^-$	7.899E-14	1.009	1.977E5	18.0	e	43
(10)	$\sigma^- + C_2F_4 \rightarrow F^- + CF_2 + CF_3$	2.514E-7	-0.6587	-6.847E4	2.5	d,f,g	42
(11)	$e^- + CF_4 \rightarrow CF_4 + e^-$	6.423E-7	-0.3186	3.999E3	0.11	V3*	44
(12)	$e^- + CF_a \rightarrow CF_a + e^-$	9.884E-9	-0.2602	1.168E3	0.05	V4 <sup>b</sup>	44
(13)	$e^- + CF_4 \rightarrow CF_4 + e^-$	0.2	-1.367	7.734E4	4.0	V*	44
(14)	$e^- + CF_4 \rightarrow CF_4 + F + e^-$	1.190E-16	1.309	1.446E5	5.6	i	44, Table 2
(15)	$e^- + CF_s \rightarrow CF_s + 2F + e^-$	7.775E-17	1.184	1.663E5	9.5	iji	44, Table 2
(16)	e + CF <sub>e→</sub> CF+3F+e	1.039E-16	1.187	2.203E5	14.9	ij	44. Table 2
(17)	e"+CF,-+CF;+F+2e"	1.159E-11	0.7645	1.993E5	15.9	-	44, Table 1:
(18)	e + CF <sub>4</sub> →CF <sub>4</sub> +2F+2e	2.886E-11	0.5108	2.649E5	22.0	1	44, Table 1
(19)	$e^- + CF_a \rightarrow CF^+ + 3F + 2e^-$	2.296E-14	1.090	3.132E5	27.0	i	44, Table 1
(20)	e + CF <sub>4</sub> →F++CF <sub>3</sub> +2e	1.482E-13	0.9375	4.023E5	23.1	i	44, Table 1
(21)	$e^- + CF_4 \rightarrow F^+ + CF_4^+ + 3e^-$	3.614E-17	1.413	3.966E5	36.0		44, Table 1
(22)	e + CF, +F++CF; +F+3e	1.809E-22	2.431	3.912E5	40.0		44, Table 1
(23)	$e^{-} + CF_4 \rightarrow F^{+} + CF^{+} + 2F + 3e^{-}$	4.867E-30	3.880	3.531E5	42.0	i	44. Table 1
(24)	e"+CF4→CF3+F"	2.369E-8	-0.4893	5.876E4	3.0	£	44, Fig. 34
(25)	$\sigma^- + CF_1 \rightarrow CF_2 + F + \sigma^-$	4.163E-4	-0.9407	1.301E5	3.8	i	46
(26)	e-+CF <sub>1</sub> →CF <sub>1</sub> +2e-	1.4E-11	0.6481	1.133E5	10.0	k	44, 47
(27)	e + CF, → CF; +F+2e	1.378E-10	0.4367	1.987E5	17.1		44, 47
(28)	e"+CF+→CF"+2F+2e"	5.005E-11	0.5060	2.455E5	21.4		44, 47
(29)	e"+CF <sub>1</sub> →F"+CF <sub>2</sub> +2e"	5.581E-10	0.2896	3.336E5	21.3	4	44, 47
(30)	e + CF <sub>1</sub> →F + CF <sub>2</sub> +2e e + CF <sub>1</sub> →CF <sub>2</sub> +F	2.369E-8	-0.4893	5.876E4	0.40	fi	copy CF4
(31)	e + CF, → CF, + e -	3.419E-4	-0.8606	9.01E4	5.6	EA 'B.	45 45
(32)	e"+CF <sub>1</sub> →CF <sub>2</sub> +e"	1.795E-4	-0.838	4.225E4	2.2	E a B c	45
(33)	e + CF <sub>2</sub> CF <sub>2</sub> +e e + CF <sub>2</sub> CF+F+e	1.795E-4 1.190E-16	1.309	1.446E5	5.4	i a bi	
(34)	e + CF <sub>2</sub> →CF+++e e - + CF <sub>3</sub> →CF++2e		0.6287	1.125E5	10.0		copy CF <sub>4</sub> 44, 47
(35)	e"+CF <sub>2</sub> →CF <sub>2</sub> +2e e"+CF <sub>2</sub> →CF"+F+2e"	1.579E-11 2.454E-12	0.0287	1.602E5	14.23		44, 47
	e + CF <sub>2</sub> →CF +F+2e e + CF <sub>2</sub> →F + CF+2e		0.7803	4.446E5	22.9	4	
(36)	e +CF2→F'+CF+Ze	1.676E-9			1.9		44, 47
(37)	e - + CF <sub>2</sub> →CF+F-	2.369E-8	-0.4893	5.876E4		f,i	copy CF4
(38)	e " + CF → C + F + e "	1.190E-16	1.309	1.446ES	5.6	i	copy CF4
(39)	e" + CF→CF" + 2e"	1.270E-13	1.038	1.027E5	9.11		47
(40)	$e^- + CF \rightarrow C + F^-$	2.369E-8	-0.4893	5.876E4	2.1	£i	copy CF4
(41)	$e^- + C \rightarrow e^- + C$	4.882E-6	-0.5042	2.459E4	1.264	E 1Dc	49
(42)	e"+C→e"+C	6.939E-7	-0.5041	4.163E4	2.684	E 150	49
(43)	e-+F→e-+F	1.56E6	-0.6504	1.663E5	12.7	E 3s *P+1	50
(44)	e"+F→e"+F	5.93E-9	-0.0528	1.605E5	12.985	E 3s <sup>2</sup> P <sup>4</sup>	50
(45)	e - + F → F + 2 e -	7.489E-13	0.8595	2.042E5	17.42		51
(46)	$e^- + SiF_4 \rightarrow SiF_4 + e^-$	4.78E-3	-1.351	4.704E3	0.032	V*	46
(47)	$e^- + SiF_4 \rightarrow SiF_4 + e^-$	4.73E-3	-1.35	4.799E3	0.052	V <sup>b</sup>	46
(48)	$e^- + SiF_4 \rightarrow SiF_4 + e^-$	2.947E-6	-0.4119	4.606E3	0.10	$V_{\theta}$	46
(49)	$e^- + SiF_4 \rightarrow SiF_5 + F + e^-$	2.268E-12	0.8182	1.302E5	7.25	i	46
(50)	$e^- + SiF_4 \rightarrow SiF_2 + 2F + e^-$	1.223E-8	0.018 34	1.86E5	11.9	i,j	46
(51)	$e^- + SiF_4 \rightarrow SiF + 3F + e^-$	1.039E-16	1.187	2.203E5	18.6	ij	copy CF4
(52)	$e^- + SiF_4 \rightarrow SiF_5^+ + 2e^- + F$	2.291E-11	0.6641	2.022E5	16.0		46
(53)	$e^- + SiF_4 \rightarrow SiF_2^+ + 2F + 2e^-$	2.886E-11	0.5108	2.649E5	23.4	i,j	copy CF4
(54)	$e^- + SiF_4 \rightarrow SiF^+ + 3F + 2e^-$	2.296E-14	1.090	3.132E5	25.1	i,j	copy CF4
(55)	$\sigma^- + SiF_4 \rightarrow F^+ + SiF_3 + 2\sigma^-$	1.482E-13	0.9375	4.023E5	24.75	i	copy CF4
(56)	$\sigma^- + SiF_4 \rightarrow SiF_5 + F^-$	1.245E-8	-0.3792	1.14E5	3.8	i	46
(57)	$e^- + SiF_3 \rightarrow SiF_2 + F + e^-$	1.190E-16	1.309	1.446E5	4.6	i	copy CF4
(58)	$e^- + SiF_1 \rightarrow SiF + 2F + e^-$	1.039E-16	1.187	2.203E5	11.4	ij	copy CF4
	$e^- + SiF_i \rightarrow SiF_i^+ + 2e^-$	3.265E-10	0.3633	1.185E5	9.60		53
(59)							
(59)	$e^- + SiF_3 \rightarrow SiF_3^+ + F + 2e^-$	1.939E-10	0.4660	1.752E5	15.90		53

	Reaction	A	В	C	6	Notes	Reference
(62)	$e^- + SiF_4 \rightarrow Si^+ + 3F + 2e^-$	1.801E-10	0.3139	3.343E5	25.6	i,j	53
(63)	$e^- + SiF_1 \rightarrow SiF_2 + F^-$	1.245E-8	-0.3792	1.14E5	3.0		copy SiF.
(64)	$e^- + SiF_2 \rightarrow SiF + F + e^-$	1.190E-16	1.309	1.446E5	6.8	i	copy CF4
(65)	$e^- + SiF_2 \rightarrow SiF_2^+ + 2e^-$	2.620E-9	0.2530	1.348E5	10.80		54
(66)	$e^- + SiF_2 \rightarrow SiF^+ + F + 2e^-$	3.597E-13	0.9855	1.592E5	15.2		54
(67)	$e^- + SiF_2 \rightarrow Si^+ + 2F + 2e^-$	7.940E-11	0.4722	3.459E5	22.4		54
(68)	$e^- + SiF_2 \rightarrow SiF + F^-$	1.245E-8	-0.3792	1.14E5	3.0		copy SiF.
(69)	$e^- + SiF \rightarrow Si + F + e^-$	1.190E-16	1.309	1.446E5	6.0	i	copy CF4
(70)	$e^- + SiF \rightarrow SiF^+ + 2e^-$	2.963E-9	0.3258	9.052E4	7.26		55
(71)	$e^- + SiF \rightarrow Si^+ + F + 2e^-$	3.888E-10	0.4391	1.628E5	14.3		55
(72)	$e^- + SiF \rightarrow Si + F^+ + 2e^-$	7.116E-11	0.3962	2.580E5	23.1		55
(73)	$e^- + SiF \rightarrow Si + F^-$	1.245E-8	-0.379	1.14E5	3.0		copy StF,
(74) (75)	e"+O2→O2+e"	3.1064E-7	-0.967 -1.02	-2.214E4 5.332E4	0.19	V, part 1 <sup>m</sup>	57 57
(76)	$e^{-} + O_{2} \rightarrow O_{2} + e^{-}$ $e^{-} + O_{3} \rightarrow O_{3} + e^{-}$	3.070E-4	-0.9297	5.65E4	0.19	V, part 2 <sup>m</sup>	57
(77)	e +02→02+e	4.792E-5 2.987E-4	-1.133	5.656E4	0.57	Va.	57
(78)	$\sigma^- + O_2 \rightarrow O_2 + \sigma^-$ $\sigma^- + O_3 \rightarrow O_3 + \sigma^-$	1.88E-3	-1.133	5.662E4	0.37	A.	57
(79)	e +O2→O2+e	1.426E-6	-0.5896	5.782E4	0.98	E σ <sup>1</sup> Δ°	57
(80)	e^++O <sub>2</sub> →O <sub>2</sub> +e	3.020E-7	-0.5739	6.214E4	1.63	Eb1X1	57
(81)	σ"+02→02+σ"	2.288E-10	0.4019	6.865E4	6.2	E° Z,	56
(82)	e"+02-02+e"	1.88E-3	-1.267	5.466E4	4.5	P	57
(83)	e-+02→0+0+e-	4.854E-7	-0.4485	5.719E4	6.0	P	57
(84)	e-+00+0+e-	4.247E-10	0.3654	5.611E4	8.4	p	57
(85)	e-+0,→0+0+e-	1.703E-16	1.29	7.557E4	10.0	P	57
(86)	e-+0,-0+0+e-	8.486E-16	1.121	7.535E4	14.7	p	57
(87)	e-+00++2e-	1.404E-15	1.419	6.549E4	12.1		57
(88)	e-+0-0+e-	9.606E-7	-0.4471	5.505E4	1.97	E1De	59
(89)	e"+0→0+e"	2.736E-8	-0.3368	6.291E4	4.19	E1Se	59
(90)	e <sup>-</sup> +0→0 <sup>+</sup> +2e <sup>-</sup>	2.314E-15	1.328	6.65E4	13.6		59
(91)	e-+CO→CO+e-	0.065 64	-1.434	2.253E4	0.27	$V^{b}$	60
(92)	e <sup>-</sup> +CO→CO+e <sup>-</sup>	0.033 33	-1.433	2.149E4	0.53	V <sup>a</sup>	60
(93)	e-+CO→CO+e-	0.013 19	-1.421	2.077E4	0.79	Va	60
(94)	e-+CO→CO+e-	0.0136	-1.471	2.149E4	1.04	V <sup>a</sup>	60
(95)	e^+CO→e^+CO	4.056E-5	-0.647	9.68E4	6.22	Ea <sup>3</sup> H;	60
(96)	e"+C0→e"+C0	5.203E-4	-0.9815	1.35E5	6.8	Ea <sup>-3</sup> Σ +c	60
(97)	e"+C0→e"+C0	1.742E-6	-0.3538	1.776E5	7.9	EA <sup>1</sup> II <sup>e</sup>	60
(98)	e"+CO→e"+CO	6.127E-5	-0.8693	1.685E5	10.4	$Eb^3\Sigma^{+e}$	60
(99)	e^+CO→e^+CO	4.756E-7	-0.2813	2.052E5	10.6	EC <sup>1</sup> Σ <sup>+</sup> +	60
(100)	e-+CO→C+O+e-	3.70E-12	0.731	1.258E Ato	mistic mo	deling - Ab-Ir	itio 1
(101)	e-+CO→CO++2e-	2.199E-7	-0.0487	2.762E5	14.0		62
	Dissociative recombinations						
(102)	$e^- + CF_1^+ \rightarrow CF_2 + F$	4.0E-8	0.0	0.0	0.0		Estimate
(103)	$e^- + CF_2^+ \rightarrow CF + F$	4.0E-8	0.0	0.0	0.0		Estimate
(104)	$\sigma^- + CF^+ \rightarrow C + F$	4.0E-8	0.0	0.0	0.0		Estimate
(105)	$e^- + SiF_3^+ \rightarrow SiF_2 + F$	4.0E-8	0.0	0.0	0.0		Estimate
(106)	$e^- + SiF_2^+ \rightarrow SiF + F$	4.0E-8	0.0	0.0	0.0		Estimate
(107)	$e^- + SiF^+ \rightarrow Si + F$	4.0E-8	0.0	0.0	0.0		Estimate
(108)	e-+CO+→C+O	4.0E-8	0.0	0.0	0.0		Estimate
(109)	$e^- + O_2^+ \rightarrow 2O$	4.0E-8	0.0	0.0	0.0		Estimate
	Detachment reactions						
(110)	$F^-+CF_3\rightarrow CF_4+e^-$	4.0E-10	0.0	0.0			Estimate
(111)	$F^-+CF_2\rightarrow CF_3+\sigma^-$ $F^-+CF\rightarrow CF_2+\sigma^-$	3.0E-10	0.0	0.0			Estimate
(112)		2.0E-10	0.0	0.0			Estimate
(113)	F +C→CF+e F +F→2F+e	1.0E-10 1.0E-10	0.0	0.0			Estimate Estimate
(114)	$F^-+F \rightarrow 2F + e^-$ $F^-+SiF_q \rightarrow SiF_q + e^-$	1.0E-10 4.0E-10	0.0	0.0		j	Estimate
(115)	F +SiF <sub>2</sub> →SiF <sub>4</sub> + e F +SiF <sub>2</sub> →SiF <sub>3</sub> + e		0.0	0.0			Estimate
(117)	$F^-+SiF_2 \rightarrow SiF_3 + e^-$ $F^-+SiF \rightarrow SiF_2 + e^-$	3.0E-10 2.0E-10	0.0	0.0			Estimate
(117)	F +SiF→SiF <sub>2</sub> +e F-+Si→SiF+e-	1.0E-10	0.0	0.0			Estimate
(119)	F +31→31F+e F +0→F+0+e	1.0E-10 1.0E-10	0.0	0.0			Estimate
(112)	Charge exchange reactions	1.0E-10	0.0	0.0		q	netimate
(120)	$O^+ + O_2 \rightarrow O_2^+ + O$	2.10E-11	0.0	0.0			63

Reaction No.	Reaction	A	В	C		Notes	Referenc
(121)	$F^++O_2 \rightarrow O_2^++F$	7.007E-10	0.0	0.0			63
(122)	Ion—ion neutralization $F^-+CF_1^+\rightarrow 2F+CF_2$	4.0E-7	-0.5	0.0			Estimate
(123)	$F^-+CF_2^+ \rightarrow F^+CF_2$ $F^-+CF_2^+ \rightarrow F^+CF_2$	4.0E-7	-0.5	0.0			Estimate
(124)	F-+CF+→2F+C	4.0E-7	-0.5	0.0			Estimate
(125)	F-+F+→2F	4.0E-7	-0.5	0.0			Estimate
(126)	$F^-+Si^+\rightarrow F+Si$	4.0E-7	-0.5	0.0			Estimate
(127)	$F^-+SiF^+ \rightarrow F+SiF$	4.0E-7	-0.5	0.0			Estimate
(128)	$F^-+SiF_2^+ \rightarrow 2F+SiF$	4.0E-7	-0.5	0.0			Estimate
(129)	$F^-+SiF_3^+ \rightarrow 2F+SiF_2$	4.0E-7	-0.5	0.0			Estimate
(130)	F +O+→F+O	4.0E-7	-0.5	0.0			Estimate
(131)	$F^-+O_2^+ \rightarrow F+O_2$	4.0E-7	-0.5	0.0			Estimate
(132)	F"+CO"→F+CO	4.0E-7	-0.5	0.0			Estimate
TABLE IV. (Contin Reaction No.	Reactio		A		С	A <sup>b</sup>	Not
(50)	$Si+SiO_2=F_2(S)\rightarrow SiF_2+$		0.04		0.0		S
(51)	$SiF+SiO_2\_F_2(S) \rightarrow SiF_1$		0.03		0.0		S
(52)	$SiF_2+SiO_2\_F_2(S)\rightarrow SiF$		0.02		0.0		S Sh
(53)	$SiF_3+0.5SiO_2\_F_2(S) \rightarrow C+SiO_4\_F_4(S) \rightarrow CF_4+$	S1F4+0.3S1O2(S)	0.01		0.0		S*

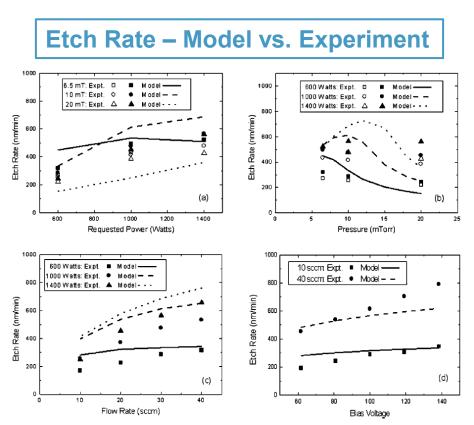
Reaction No.	Reaction	A	C	hb	Note
	Direct etch by F atoms				
(1)	$F+0.25SiO_2(B)\rightarrow 0.25SiF_4+0.25O_2$	0.015 82	1890		S4
	Adsorption of radicals				
(2)	$F+0.5SiO_2(S)\rightarrow 0.5SiO_{2m}F_2(S)$	0.02	0.0		Salf
(3)	$CF_2+SiO_2(S)\rightarrow SiO_2\_CF_2(S)$	0.66	0.0		S#
(4)	$CF_1+1.5SiO_2(S) \rightarrow SiO_2\_CF_2(S)+0.5SiO_2\_F_2(S)$	0.2	0.0		2*a
(5)	$CF+0.5SiO_2\_F_2(S)+0.5SiO_2(S) \rightarrow SiO_2\_CF_2(S)$	1.0	0.0		Sea
	Ion-enhanced etch				
(6)	$CF_2^+ + e^- + \#SiO_2(B) + 2\#SiO_2 - F_2(S) \rightarrow CF_2 + \#SiF_4 + \#O_2 + 2\#SiO_2(S)$	1.0	0.0	0.066	B <sub>b</sub>
(7)	$CF_{3}^{+} + \sigma^{-} + \#SiO_{2}(B) + 2\#SiO_{2} - F_{2}(S) \rightarrow CF_{3} + \#SiF_{4} + \#O_{2} + 2\#SiO_{2}(S)$	1.0	0.0	0.092	By Br
(8)	$CF^+ + \sigma^- + \#SiO_2(B) + 2\#SiO_2 - F_2(S) \rightarrow CF + \#SiF_4 + \#O_2 + 2\#SiO_2(S)$	1.0	0.0	0.041	By Br
(9)	$F^+ + \sigma^- + \# SiO_2(B) + 2\# SiO_2 = F_2(S) \rightarrow F + \# SiF_4 + \# O_2 + 2\# SiO_2(S)$	1.0	0.0	0.025	B <sub>7</sub> B <sub>4</sub>
	$Si^+ + \sigma^- + \#SiO_2(B) + 2\#SiO_3 - F_2(S) \rightarrow Si + \#SiF_4 + \#O_2 + 2\#SiO_2(S)$		0.0		B <sub>p</sub>
(11)	$SiF^+ + \sigma^- + \#SiO_2(B) + 2\#SiO_2 - F_2(S) \rightarrow SiF + \#SiF_4 + \#O_2 + 2\#SiO_2(S)$	1.0	0.0	0.062	By Br
(12)	$SiF_2^+ + \sigma^- + \# SiO_3(B) + 2\# SiO_3 - F_2(S) \rightarrow SiF_2 + \# SiF_4 + \# O_3 + 2\# SiO_2(S)$ $SiF_4^+ + \sigma^- + \# SiO_4(B) + 2\# SiO_4 - F_4(S) \rightarrow SiF_4 + \# SiF_4 + \# O_4 + 2\# SiO_4(S)$	1.0			B <sub>2</sub>
			0.0	0.113	By Br
(14)	$O^{+}+\sigma^{-}+\sharp SiO_{2}(B)+2\sharp SiO_{2}\_F_{2}(S)\longrightarrow O+\sharp SiF_{4}+\sharp O_{2}+2\sharp SiO_{2}(S)$	1.0	0.0	0.021	By Br
(15)	$O_2^+ + \sigma^- + \# SiO_2(B) + 2\# SiO_2 - F_2(S) \rightarrow O_2 + \# SiF_4 + \# O_2 + 2\# SiO_2(S)$	1.0			By Br
(16)	$CO^{+} + e^{-} + \$ SiO_{2}(B) + 2SiO_{2} - F_{2}(S) \rightarrow CO + \$ SiF_{4} + \$ O_{2} + 2\$ SiO_{2}(S)$	1.0	0.0	0.037	
(17)	$CF_2^+ + \sigma^- + \#SiO_2(B) + 2\#SiO_2 - CF_2(S) \rightarrow CF_2 + \#SiF_4 + 2\#CO + 2\#SiO_2(S)$	1.0	0.0	0.067	Bi Bi
(18)	$CF_3^+ + e^- + \sharp SiO_2(B) + 2\sharp SiO_2 - CF_2(S) \rightarrow CF_3 + \sharp SiF_4 + 2\sharp CO + 2\sharp SiO_2(S)$	1.0	0.0	0.093	
(19)	$CF^+ + e^- + \#SiO_2(B) + 2\#SiO_2 - CF_2(S) \rightarrow CF + \#SiF_4 + 2\#CO + 2\#SiO_2(S)$	1.0	0.0	0.042	Bi
(20)	$F^+ + e^- + \#SiO_2(B) + 2\#SiO_2 - CF_2(S) \rightarrow F + \#SiF_4 + 2\#CO + 2\#SiO_2(S)$	1.0	0.0	0.026	B <sup>1</sup>
(21)	$Si^+ + e^- + \#SiO_2(B) + 2\#SiO_2 - CF_2(S) \rightarrow Si + \#SiF_4 + 2\#CO + 2\#SiO_2(S)$	1.0	0.0	0.038	B <sup>1</sup>
(22)	$SiF^+ + e^- + \#SiO_2(B) + 2\#SiO_2 - CF_2(S) \rightarrow SiF + \#SiF_4 + 2\#CO + 2\#SiO_2(S)$	1.0	0.0	0.063	B <sup>1</sup>
(23)	$SiF_2^+ + e^- + \#SiO_2(B) + 2\#SiO_2 - CF_2(S) \rightarrow SiF_2 + \#SiF_4 + 2\#CO + 2\#SiO_2(S)$	1.0	0.0	0.090	B
(24)	$SiF_1^+ + e^- + \#SiO_2(B) + 2\#SiO_2 - CF_2(S) \rightarrow SiF_3 + \#SiF_4 + 2\#CO + 2\#SiO_2(S)$	1.0	0.0	0.116	B <sup>i</sup>
(25)	$O^+ + e^- + $SiO_2(B) + 2$SiO_2\_CF_2(S) \rightarrow O + $SiF_4 + 2$CO + 2$SiO_2(S)$	1.0	0.0	0.021	B
(26)	$O_2^+ + e^- + $SiO_2(B) + 2$SiO_2 - CF_2(S) \rightarrow O_2 + $SiF_4 + 2$CO + 2$SiO_2(S)$	1.0	0.0	0.044	B <sup>i</sup>
(27)	$CO^{+} + e^{-} + \sharp SiO_{2}(B) + 2\sharp SiO_{2}CF_{2}(S) \rightarrow CO + \sharp SiF_{4} + 2\sharp CO + 2\sharp SiO_{2}(S)$	1.0	0.0	0.038	B <sup>i</sup>
	Ion neutralization on open sites				
(28)	$CF_3^+ + e^- + SiO_2(S) \rightarrow CF_3 + SiO_2(S)$	0.8	0.0		В
(29)	$CF_2^+ + e^- + SiO_2(S) \rightarrow CF_2 + SiO_2(S)$	0.8	0.0		В
(30)	$CF^++e^-+SiO_2(S)\rightarrow CF+SiO_2(S)$ [No Title]	0.8	0.0		В
(31)	$F^++e^-+SiO_2(S)\rightarrow F+SiO_2(S)$	0.8	0.0		В
(32)	$Si^+ + e^- + SiO_2(S) \rightarrow Si + SiO_2(S)$	1.0	0.0		В
(33)	$SiF^+ + e^- + SiO_2(S) \rightarrow SiF + SiO_2(S)$	0.8	0.0		В
(34)	$SiF_2^+ + e^- + SiO_2(S) \rightarrow SiF_2 + SiO_2(S)$	0.8	0.0		В
(35)	$SiF_3^+ + e^- + SiO_2(S) \rightarrow SiF_3 + SiO_2(S)$	0.8			В
(36)	$O^{+}+e^{-}+SiO_{2}(S)\rightarrow 0.5O_{2}+SiO_{2}(S)$	1.0	0.0		В
(37)	$O_2^+ + \sigma^- + SiO_2(S) \rightarrow O_2 + SiO_2(S)$	1.0	0.0		B B
(38)	$CO^+ + e^- + SiO_2(S) \rightarrow CO + SiO_2(S)$	1.0	0.0		В
1200	Ion deposition reactions				Total Control
(39)	$CF_1^+ + e^- + 1.5SiO_2(S) \rightarrow SiO_2 - CF_2(S) + 0.5SiO_2 - F_2(S)$	0.2	0.0		B,
(40)	$CF_2^+ + e^- + SiO_2(S) \rightarrow SiO_2 \_CF_2(S)$	0.2	0.0		B*
(41)	$CF^+ + e^- + SiO_2 - F_2(S) + 0.5SiO_2(S) \rightarrow SiO_2 - CF_2(S) + 0.5SiO_2 - F_2(S)$		0.0		B.
(42)	$F^+ + e^- + 0.5SiO_2(S) \rightarrow 0.5SiO_2 - F_2(S)$	0.2			
(43)	$SiF^+ + e^- + 0.5SiO_2(S) \rightarrow Si + SiO_2 - F_2(S)$	0.2	0.0		B*
(44)	$SiF_2^+ + e^- + SiO_2(S) \rightarrow Si + SiO_2 - F_2(S)$	0.2	0.0		B,
(43)	$SiF_1^+ + e^- + 1.5SiO_2(S) \rightarrow Si + 1.5SiO_2 - F_2(S)$ Radical abstraction/recombination reactions at surface	0.2	0.0		В.
(46)	F+0.5SiO₁_CF₁(S)→0.5CF₄+0.5SiO₁(S)	0.01	0.0		St
(47)	$Si+SiO_3$ _ $CF_3(S) \rightarrow CF+SiF+SiO_3(S)$	0.04	0.0		s
(48)	$SiF+SiO_1\_CF_2(S) \rightarrow SiF_2+CF+SiO_2(S)$	0.03	0.0		s



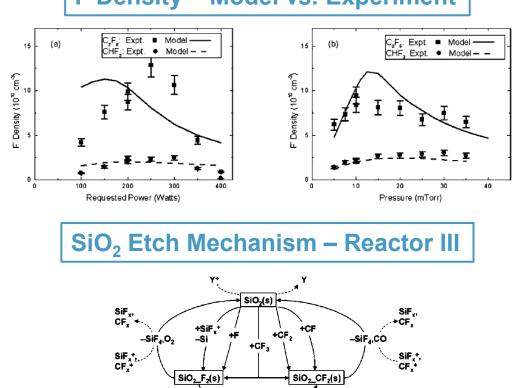


## Ho – SiO<sub>2</sub> Etch in C<sub>2</sub>F<sub>6</sub> Plasma – Comparison to Experiments

- Ho et al. compared their 0D modeling results to a wide variety of experimental data:
  - ► SiO<sub>2</sub> etch rate over a range of conditions in 2 chambers
  - ► F, SiF, and CF<sub>x</sub> radical densities
  - Electron density



## F Density – Model vs. Experiment



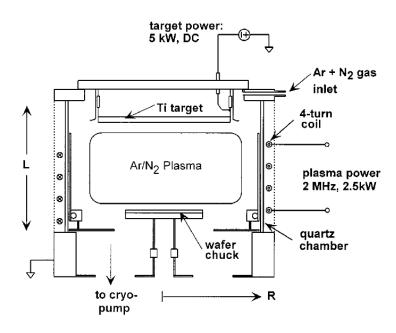
Adsorption and Etching Reactions ----- Concomitant Ion Reactions



#### Tao – Ionized PVD of TiN – Model

- Tao, Mao, and Hopwood developed a global model for TiN ionized physical vapor deposition (IPVD).
- Model targeted towards 1 experimental system.
- Plasma chemistry is relatively simple with important Ar, N and Ti species included.
- Assumptions: volume averaged densities, sputtered Ti fully thermalized, TiN forms on surface.

#### TiN IPVD Reactor



#### Ti/Ar/N<sub>2</sub> Plasma Chemistry

Reaction	Rate constants	Reference
$ \overline{\mathbf{N} + e^- \rightarrow \mathbf{N}^+ + 2e^-} $	$K_1 = 3.84 \times 10^{-9} (T_e)^{0.92} \exp(-12.1/T_e) \text{ cm}^3 \text{ s}^{-1}$	a
$N_2 + e^- \rightarrow N_2^+ + 2e^-$	$K_2 = 1.95 \times 10^{-9} (T_e)^{1.13} \exp(-14.4/T_e) \text{ cm}^3 \text{ s}^{-1}$	b
$N_2 + e^- \rightarrow 2N + e^-$	$K_3 = 6.15 \times 10^{-9} (T_e)^{0.81} \exp(-12.8/T_e) \text{ cm}^3 \text{ s}^{-1}$	c
$N^+ + N_2 \rightarrow N_2^+ + N$	$K_5 = 2.0 \times 10^{-11} \text{ cm}^3 \text{ s}^{-1}$	d
$N+N_2^+ \to N^+ + N_2$	$K_6 = 1.0 \times 10^{-11} \text{ cm}^3 \text{ s}^{-1}$	e
$N_2^* + N \rightarrow N + N_2$	$K_7 = 4.0 \times 10^{-11} \text{ cm}^3 \text{ s}^{-1}$	f
$N_2^* + N_2 \rightarrow 2N_2$	$K_8 = 3.5 \times 10^{-12} \text{ cm}^3 \text{ s}^{-1}$	g
$N_2 + e^- \rightarrow N_2^* + e^-$	$K_9 = 5.81 \times 10^{-9} \exp(-7.57/T_e) \text{ cm}^3 \text{ s}^{-1}$	h
$N_2^* \rightarrow N_2 + h \nu$	$\tau_{h\nu} = 2.3 \times 10^{-4} \text{ s}$	g
$N(\text{wall}) \rightarrow \frac{1}{2} N_2(g)$	$ au_{ m N}^{-1} \! = \! D_{ m N} / \Lambda_{ m N}^2  { m s}^{-1}$	i
$Ar^{+}\overrightarrow{+N_{2}} \rightarrow N_{2}^{+} + Ar$	$K_{10} = 1.2 \times 10^{-11} \text{ cm}^3 \text{ s}^{-1}$	j
$Ar + e^- \rightarrow Ar^* + e^-$	$K_{11} = 2.2 \times 10^{-8} \exp(-12.4/T_e) \text{ cm}^3 \text{ s}^{-1}$	k
$Ar^* + e^- \rightarrow Ar^+ + 2e^-$	$K_{12} = 2.1 \times 10^{-7} \exp(-5.3/T_e) \text{ cm}^3 \text{ s}^{-1}$	1
$Ar+e^- \rightarrow Ar^+ + 2e^-$	$K_{13} = 1.23 \times 10^{-7} \exp(-18.68/T_e) \text{ cm}^3 \text{ s}^{-1}$	m
$Ti+e^- \rightarrow Ti^+ + 2e^-$	$K_{14} = 2.34 \times 10^{-7} \exp(-7.25/T_e) \text{ cm}^3 \text{ s}^{-1}$	n
$Ti + Ar^* \rightarrow Ti^+ + Ar + e^-$	$K_{15} = \sigma_{\text{Ti}} \cdot \nu_{\text{th}_{-}\text{Ti}} \text{ cm}^3 \text{ s}^{-1}$	0



## **Tao – Ionized PVD of TiN – Comparison to Experiments**

- Tao et al. tested their model using experimental measurements in the IPVD chamber.
- Decent model experiment agreement achieved.
- Assumed different sticking coefficient for N at low and high N<sub>2</sub> flows to explain experimental observation.

#### 0.65 ▼ 1500W (experiment) 1250W (experiment) 0.60 1000W (experiment) 0.55 750W (experiment) 0.50 0.45 0.40 0.35 0.30 0.30 0.25 0.20 0.15 0.10 5sccm N<sub>a</sub> + 50 sccm Ar 0.05 0.00 15mTorr 20mTorr 25mTorr 30mTorr Pressure (mTorr)

FIG. 3. Comparison of the experimental dissociation of nitrogen (symbols) and the computed dissociation (solid lines).

#### **TiN IPVD Model – Experiment Comparison**

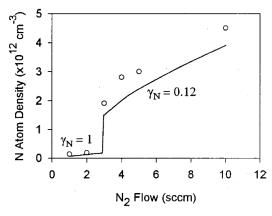


FIG. 4. The modeled atomic nitrogen density (solid line) is compared with experimental measurements ( $\bigcirc$ ) described in Ref. 11. The increase in [N] at 3 sccm is due to the experimentally observed transition from the metal target mode to the nitride target mode. The transition is modeled by decreasing the N wall loss parameter from  $\gamma_N$ = 1 to  $\gamma_N$ = 0.12. Plasma conditions were 15 mTorr total pressure, 1 kW plasma power, and 1 kW target power.

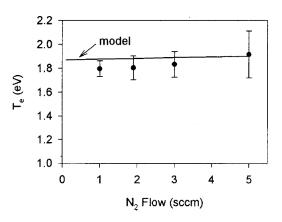


FIG. 5. Comparison of computed and measured electron temperature.

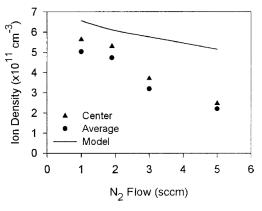


FIG. 6. Comparison of the computed global ion density with the ion density measured at the center of the discharge and the average ion density.



## Liang – 60 MHz N<sub>2</sub> Capacitively Coupled Plasma – Model

- Liang et al. developed a 2D fluid model of N<sub>2</sub> capacitively coupled plasma (CCP) operating at 60 MHz.
- The model was tested against experimentally measured N<sub>2</sub><sup>+</sup> ion density.
- Model was used to understand the effect of RF power and inter-electrode gap on plasma uniformity.

## **60 MHZ CCP** Gas inlet Matching 60MHz network rf source Oscilloscope Showerhead Data cquisition Pump out Corrugated pipe

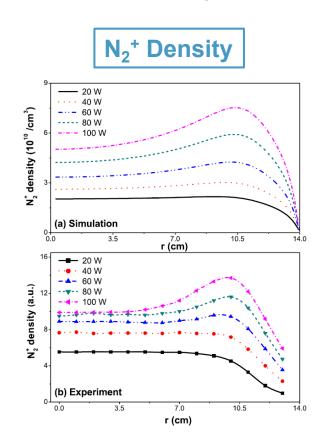
#### N<sub>2</sub> Plasma Chemistry

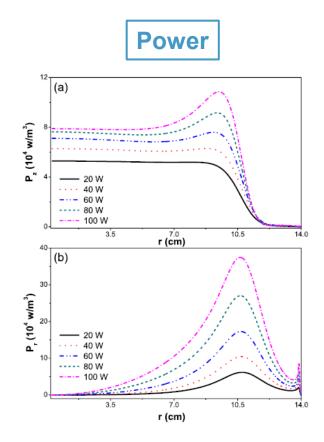
TABLE I. The reactions taken into account in the model

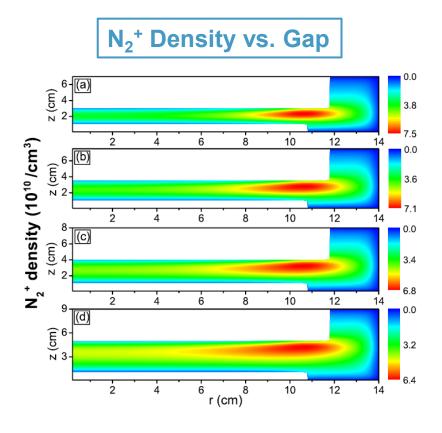
No.	Reactions	Rate Coefficient <sup>a</sup>	$\varepsilon^{\mathbf{b}}$	Reference
R1	$N_2 + e \rightarrow N_2 + e$	$1.04 \times 10^{-7} (T_e)^{0.43} \exp(-0.206/T_e)^{c}$		29
R2	$N + e \rightarrow N^+ + 2e$	$3.87 \times 10^{-9} (T_e)^{0.86} \exp(-14.62/T_e)^{c}$	14.54	29
R3	$N_2 + e \rightarrow N_2^+ + 2e$	$7.76 \times 10^{-9} (T_e)^{0.79} \exp(-16.75/T_e)^{c}$	15.60	29
R4	$N_2 + e \rightarrow N_2(A) + e$	$8.06 \times 10^{-10} (T_e)^{-0.306} \exp(-8.87/T_e)^{c}$	6.17	29
R5	$N_2 + e \rightarrow N_2(B) + e$	$1.56 \times 10^{-8} (T_e)^{-0.52} \exp(-9.16/T_e)^{c}$	7.35	29
R6	$N_2 + e \rightarrow N_2(a') + e$	$6.6 \times 10^{-9} (T_e)^{-0.66} \exp(-11.05/T_e)^{c}$	8.40	29
R7	$N_2^+ + e \rightarrow N + N$	$1.8 \times 10^{-7} (T_e)^{-0.39} \mathrm{c}$		15
R8	$N_2 + e \rightarrow N + N + e$	$2.15 \times 10^{-8} \exp(-14.39/T_e)^{c}$	9.75	30
R9	$N_2(A) + N_2(a') \rightarrow N_2^+ + N_2 + e$	$3.2 \times 10^{-12}$		31
R10	$N_2(a') + N_2(a') \rightarrow N_2^+ + N_2 + e$	$5.0 \times 10^{-11}$		32
R11	$N_2^+ + N \rightarrow N^+ + N_2$	$7.21 \times 10^{-13} \exp(T_{gas}/300.0)^{d}$		31
R12	$N_2(A) + N \rightarrow N_2 + N$	$2.0 \times 10^{-12}$		31
R13	$N_2(A) + N_2 \rightarrow N_2 + N_2$	$3.0 \times 10^{-18}$		33
R14	$N_2(A) + N_2(A) \rightarrow N_2(B) + N_2$	$7.7 \times 10^{-11}$		16
R15	$N_2(B) + N_2 \rightarrow N_2(X_{v=0}) + N_2$	$1.5 \times 10^{-12}$		34
R16	$N_2(B) + N_2 \rightarrow N_2(A) + N_2$	$2.85 \times 10^{-11}$		34
R17	$N_2(a') + N_2 \rightarrow N_2(B) + N_2$	$1.9 \times 10^{-13}$		16
R18	$N + N + N \rightarrow N_2(B) + N_2$	$8.27 \times 10^{-34} exp(500.0/T_{gas})^{d,e}$		16
R19	$N + N + N_2 \rightarrow N_2 + N$	$1.0 \times 10^{-32e}$		33
R20	$N_2(B) \rightarrow N_2(A) + h\nu$	$2.0 \times 10^{5f}$		16

## Liang – 60 MHz N<sub>2</sub> Capacitively Coupled Plasma – Plasma Uniformity

- The model showed that plasma intensified closer to the electrode edge as power increased.
- Plasma uniformity worsening with power linked to  $P_r$  at electrode edge increasing more rapidly than  $P_z$ .
- Demonstrated using model that inter-electrode gap can be increased to improve plasma uniformity.

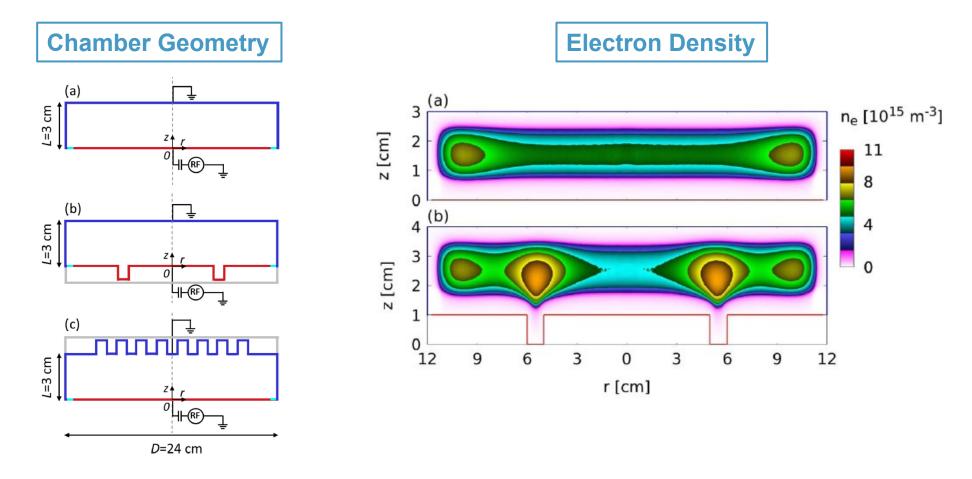






## Wang – Uniformity Control in Capacitive Discharge – Model

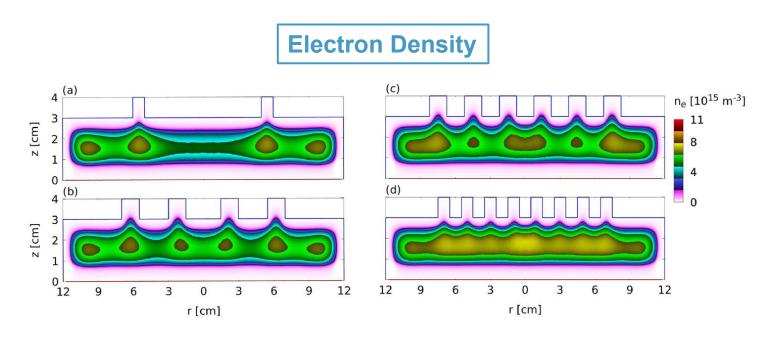
- Wang et al. used a 2D PIC/MCC model to simulate a cylindrical 13.56 MHz CCP.
- Examined the effect of introducing trenches in the top (grounded) and bottom (powered electrode).
- Simulations done for Ar plasma, 10 Pa, 1024 points in radial + axial directions, and > 7 million particles.



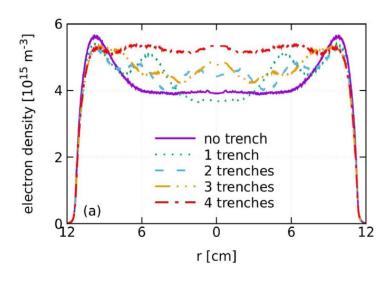


## Wang – Uniformity Control in Capacitive Discharge – Testing New Concept

- The plasma density peaked at chamber edge due to strong electron heating at powered electrode edge.
- Found that electron heating enhances near trench corners, intensifying the plasma in the trench's vicinity.
- Demonstrated that multiple ring-shaped trenches can be used to improve the plasma uniformity.



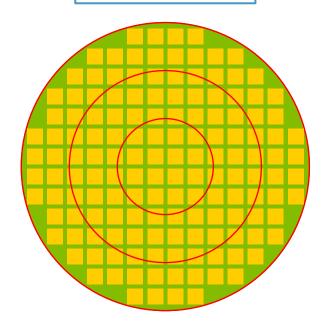
## **Electron Density vs. r**



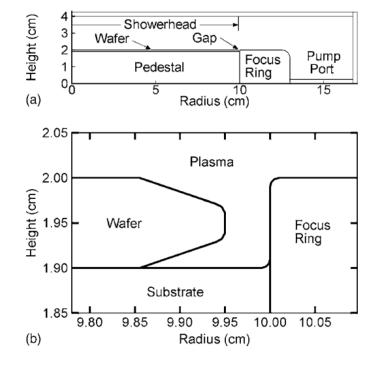
## Babaeva – Plasma at Wafer Edge – Model

- Babaeva and Kushner examined the effect of the gap between wafer and focus ring.
- 2D simulations of the CCP discharge were done using nonPDPSIM, a fluid plasma model.
- Simulations were done for Ar/CF<sub>4</sub> plasma at 90 mTorr with 10 MHz power.

#### Dies on Wafer



#### **Chamber Geometry**



#### **Ar/CF**₄ Chemistry

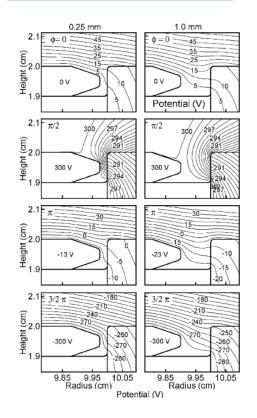
	Species	
	CF <sub>4</sub> CF <sub>3</sub>	
	CF <sub>3</sub> CF <sub>3</sub>	
	CF <sub>2</sub> F	
Ar*	CF e	
	F <sub>2</sub>	
	7	
Reactions	Rate coefficient	•
Electron Impact:	6	
$e+Ar \rightarrow Ar^*+e$		
$e+Ar \rightarrow Ar^{++}+e$		
$e+Ar \rightarrow Ar^++e+e$		
$e+Ar^+ \rightarrow Ar^+ + e+e$		
$e+Ar^* \rightarrow Ar+e$		
$e+Ar^{\circ} \rightarrow Ar^{\circ \circ}+e$	6	
$e+Ar^{**} \rightarrow Ar+e$	6	
$e+Ar^{**} \rightarrow Ar^*+e$		
e+Ar**→Ar*+e	c	
$e+CF_4 \rightarrow CF_3+F^-$		
$e+CF_4 \rightarrow CF_3 + F$		
$e+CF_4 \rightarrow CF_3+F+e$		
$e+CF_4 \rightarrow CF_3^*+F+e$		
$e+CF_4 \rightarrow CF_2+F+F$	te c	
$e+CF_4 \rightarrow CF_3^++F^-+e$		
$e+CF_4 \rightarrow CF+F+F_2$	re .	
$e+CF_3 \rightarrow CF_2+F+e$	6	
$e+CF_3 \rightarrow CF_3^*+e+e$	6	
$e+CF_3 \rightarrow CF_2+F^-$		
$e+CF_2 \rightarrow CF+F^-$	· ·	
$e+CF_2 \rightarrow CF+F+e$		
$e+F_2 \rightarrow F^-+F$		
Neutral heavy partic		
Ar°+Ar°→Ar+Ar	e 1.0×10 <sup>-9</sup>	
$Ar^{**} + Ar^{**} \rightarrow Ar^{*} + A$		
$Ar^{**} + Ar^{*} \rightarrow Ar^{*} + Ar$ $Ar^{**} \rightarrow Ar^{*}$		
	$2 \times 10^6 \text{ s}^{-1}$ $2.0 \times 10^{-11}$	
$F+CF_3 \rightarrow CF_4$		
$F+CF_2 \rightarrow CF_3$ $F+CF \rightarrow CF_2$	$1.8 \times 10^{-11}$ $9.96 \times 10^{-11}$	
	9.96 × 10 ··· 8.3 × 10 <sup>-14</sup>	
$F_2+CF_2 \rightarrow CF_3+F$		
$F_2+CF_3 \rightarrow CF_4+F$	1.88×10 <sup>-14</sup> +Ar 4.0×10 <sup>-11</sup>	
$Ar^*+CF_4 \rightarrow CF_2+F_2$		
$Ar^{\circ}+CF_3 \rightarrow CF_2+F+$ $Ar^{\circ}+CF_3 \rightarrow CF+F+$		
$Ar^{-}+CF_{2}\rightarrow CF+F+$ Ion-neutral particle		
Ar+Ar→Ar+Ar	4.6×10 <sup>-10</sup>	
$A\Gamma^+A\Gamma \rightarrow A\Gamma + A\Gamma^-$ $CF_1^++CF_3 \rightarrow CF_3+C$		
$CF_1+CF_3\rightarrow CF_3+C$ $CF_1+F\rightarrow CF_1+F$	5.0×10 <sup>-8</sup>	
$F^-+CF_1 \rightarrow CF_3+e$	4.0×10 <sup>-10</sup>	
$F^-+CF_2 \rightarrow CF_3+e$	3.0×10 <sup>-10</sup>	
$F^-+CF_2 \rightarrow CF_3+e$ $F^-+CF \rightarrow CF_3+e$	2.0×10 <sup>-10</sup>	
	1.0×10 <sup>-10</sup>	
$F^-+F \rightarrow F_2+e$		
$Ar^++CF_4 \rightarrow CF_3^++Ar$	+F 4.8×10 <sup>-10</sup> 7.0×10 <sup>-10</sup>	
$Ar^*+CF_3 \rightarrow CF_3^*+Ar$		
Electron-ion and ion		
e+Ar <sup>+</sup> →Ar <sup>**</sup>	$4.0 \times 10^{-13} T_e^{-0.5}$	
$e+CF_3^+ \rightarrow CF_2+F$	3.0 × 10 1,	
$CF_3^-+CF_3^+ \rightarrow CF_3+C$		
$F^-+CF_3^+ \rightarrow CF_2+F_2$	8.7×10 <sup>-8</sup>	0.5
$F^-+CF_3^+ \rightarrow CF_2+F+$		-
$F^-+CF_3^+ \rightarrow F+CF_3$	$3.0 \times 10^{-7}$	
$CF_1^- + Ar^+ \rightarrow CF_3 + Ar$	$3.0 \times 10^{-7}$	



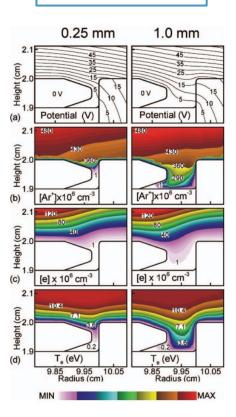
## Babaeva – Plasma at Wafer Edge – Results

- As wafer edge focus ring gap increased from  $0.25 \rightarrow 1$  mm, the plasma reached below the wafer edge.
- Demonstrated that height of focus ring can be used to control plasma penetration under the wafer edge.

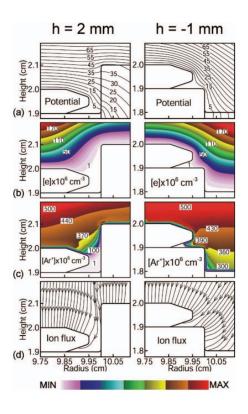
#### Potential vs. Time



## **Effect of Gap**



## **Effect of Ring Height**



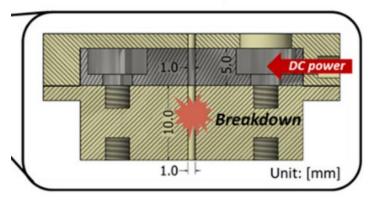


## Son – Plasma Breakdown in Narrow Gap – Model

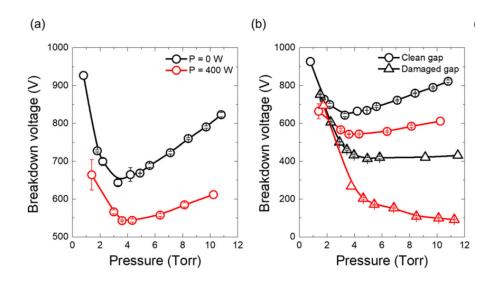
- Reliability is key for industrial products. Helping fix issues in an important part of engineers' job.
- This includes unintended gas breakdown in regions that should be plasma-free.
- Son et al. studied gas breakdown in narrow gaps which are exposed to the main plasma volume.
- EDIPIC was used to do 2D PIC/MCC simulations in Ar at 5 Torr.  $\Delta x = 5 \mu m$ ,  $\Delta t = 4 ps$ .

## **Geometry**

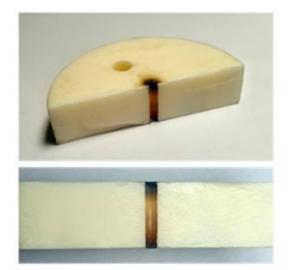
#### Modular device for plasma-facing gap Gas breakdown experiments



#### **Breakdown Voltage vs. Pressure**



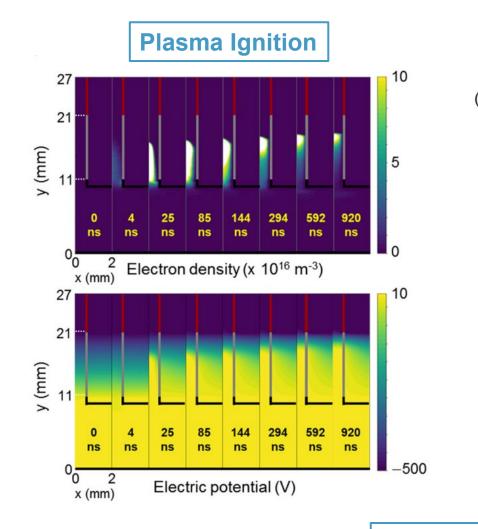
#### **Damaged Material**





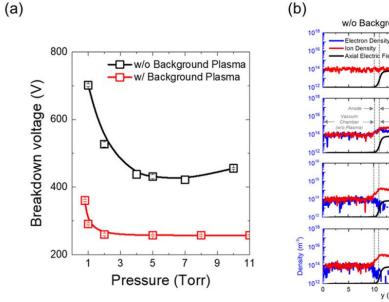
## Son – Plasma Breakdown in Narrow Gap – Results

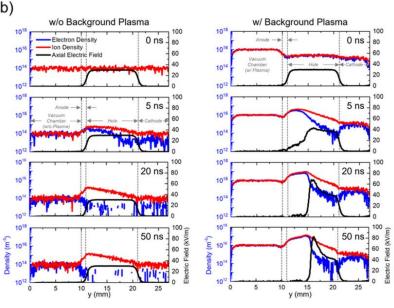
They demonstrated that presence of low-density electrons in the gap significantly lowers the breakdown voltage.









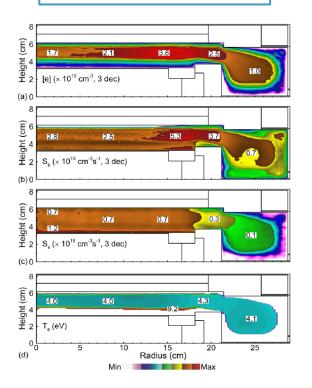




## **Huang – HAR Dielectric Etch – Model**

- Huang et al. used a coupled plasma + feature scale model to examine high aspect ratio (HAR) dielectric etch.
- Plasma model: HPEM, feature scale model: MCFPM (University of Michigan).
- The model included detailed chemistry for  $Ar/C_4F_8/O_2$  and a detailed mechanism for  $SiO_2$  etch.

## **Plasma Properties**



ions, hot neutrals, and neutral partners		Ar*, Ar(h), Ar		
•				
		F*, F(h), F		
		F2*, F2(h), F2		
		O*, O(h), O		
		O2*, O2(h), O2		
		$C_mF_n^+$ , $C_mF_n(h)$ , $C_mF_n$		
Etch products		CO, CO2, COF, COH		
		SiFx, SiF4		ь
Sputtered materials		R, SiO <sub>2</sub> , Si		
Surface sites				Not
Photoresist		R(s)		
Silicon oxide		SiO <sub>2</sub> (s)		
Passivated oxide surface (complex)		$SiO_2C_mF_n(s)$		4
		SiOCF <sub>3</sub> (s)		
Silicon		Si(s)		
Fluorinated silicon surface		SiF <sub>x</sub> (s)		
Polymer		P(s)		
Activated surface sites		SiO <sub>2</sub> *(s)		
		$SiO_2C_mF_n^{\ \ e}(s)$		
		SiOCF <sub>3</sub> *(s) P*(s)		
Reactions <sup>6</sup>	Po <sup>b</sup>	E <sub>th</sub> (eV) <sup>b</sup>	E <sub>r</sub> (eV) <sup>h</sup>	Notes
Activation of SiO <sub>2</sub>			-4(7	
SiO <sub>2</sub> (s) + I <sup>+</sup> $\rightarrow$ SiO <sub>2</sub> *(s) + I(h)	0.9			100
$Sputtering of SiO_2$	0.9			
SiO <sub>2</sub> (s) + $I^*$ $\rightarrow$ SiO <sub>2</sub> + $I(h)$	0.9	70	140	- 4
$SiO_2(s) + I^+ \rightarrow SiO_2 + I(h)$ $SiO_2^+(s) + I^+ \rightarrow SiO_2 + I(h)$	0.9	70	140	i i
Passivation of SiO <sub>2</sub>	0.9	70	140	
$SiO_2(s) + CF \rightarrow SiO_2CF(s)$	0.4			Ref. 35
$SiO_2(s) + CF_2 \rightarrow SiO_2CF_2(s)$ $SiO_2(s) + CF_2 \rightarrow SiO_2CF_2(s)$	0.3			Ref. 35
$SiO_2(s) + CF_2 \rightarrow SiO_2CF_2(s)$ $SiO_2(s) + CF_3 \rightarrow SiO_2CF_3(s)$	0.2			Ref. 35
$SiO_2(s) + CF_3 \rightarrow SiO_2CF_3(s)$ $SiO_2(s) + C_3F_3 \rightarrow SiO_2C_3F_3(s)$	0.2			Ref. 39.
$SiO_2(s) + CF_s \rightarrow SiO_2C_3(s)$ $SiO_2*(s) + CF_s \rightarrow SiO_2C_F(s)$	0.9			kd. 39,
$SiO_2^{\bullet}(s) + C_4 F_4 \rightarrow SiO_2 C_4 F_3(s)$ $SiO_2^{\bullet}(s) + C_4 F_4 \rightarrow SiO_2 C_4 F_3(s)$	0.9			k
Further passivation of complex	0.9			
SiO <sub>2</sub> CF(s) + CF <sub>2</sub> $\rightarrow$ SiO <sub>2</sub> C <sub>2</sub> F <sub>3</sub> (s)	10-4			
$SiO_2CF(s) + CF_2 \rightarrow SiO_2C_2F_3(s)$ $SiO_2CF_2(s) + CF \rightarrow SiO_2C_3F_3(s)$	10-4			
$SiO_2CF_2(s) + CF \rightarrow SiO_2C_2F_3(s)$ $SiO_2CF_2(s) + CF_2 \rightarrow SiO_2C_2F_4(s)$	10-4			
$SiO_2CF_2(s) + CF_2 \rightarrow SiO_2C_2F_4(s)$ $SiO_2CF_2(s) + C_2F_3 \rightarrow SiO_2C_3F_3(s)$	10-4			
$SiO_2CF_2(s) + C_2F_3 \rightarrow SiO_2C_3F_3(s)$ $SiO_3CF_4(s) + CF \rightarrow SiO_3C_3F_4(s)$	10-4			
$SiO_2CF_3(s) + CF \rightarrow SiO_2C_2F_4(s)$ $SiO_2CF_4(s) + C_2F_1 \rightarrow SiO_2C_1F_6(s)$	10 <sup>-4</sup>			
$SiO_2CF_3(s) + C_2F_3 \rightarrow SiO_2C_3F_6(s)$ $SiO_2C_2F_3(s) + CF_2 \rightarrow SiO_2C_3F_5(s)$	10-4			
$SiO_2C_2F_3(s) + CF_2 \rightarrow SiO_2C_3F_3(s)$ $SiO_2C_2F_4(s) + CF \rightarrow SiO_2C_3F_4(s)$	10-4			
$SiO_2C_3F_4(s) + CF \rightarrow SiO_2C_3F_3(s)$ $SiO_2C_3F_4(s) + CF_5 \rightarrow SiO_2C_3F_5(s)$	10-4			
$SiO_2C_2\Gamma_4(s) + C\Gamma_2 \rightarrow SiO_2C_3\Gamma_6(s)$ Fluorination of passivated surface	10			
SiO <sub>2</sub> CF(s) + F $\rightarrow$ SiO <sub>2</sub> CF <sub>2</sub> (s)	0.1			
$SiO_2CF_3(s) + F \rightarrow SiO_3CF_2(s)$ $SiO_2CF_3(s) + F \rightarrow SiO_3CF_3(s)$	0.1			
$SiO_2CP_2(s) + F \rightarrow SiO_2CP_2(s)$ $SiO_2C_2F_3(s) + F \rightarrow SiO_2C_2F_d(s)$	0.1			
$SiO_2C_2F_3(s) + F \rightarrow SiO_2C_2F_4(s)$ $SiO_2C_3F_4(s) + F \rightarrow SiO_2C_3F_4(s)$	0.1			
Etching of passivated surface complex	0.1			
Etching of passivated surface complex $SiO_2CF(s) + I^* \rightarrow SiF + CO_2 + I(h)$	0.75	35	140	Les.
$SiO_2CF(s) + I^- \rightarrow SiF + CO_2 + I(h)$ $SiO_2CF_2(s) + I^+ \rightarrow SiF_2 + CO_2 + I(h)$	0.75	35 35	140	100
$SiO_2CF_2(s)+I^+ \rightarrow SiF_2+CO_2+I(h)$ $SiO_2CF_3(s)+I^+ \rightarrow SiF_3+CO_2+I(h)$	0.75	35	140 140	500
	0.75	35 35	140 140	i.m
$SiO_2C_2F_3(s) + I^+ \rightarrow SiOCF_3(s) + CO + I(h)$ $SiO_2C_2F_4(s) + I^+ \rightarrow SiOCF_3(s) + COF + I(h)$	0.75	35	140	Les

## SiO<sub>2</sub> Etch Mechanism

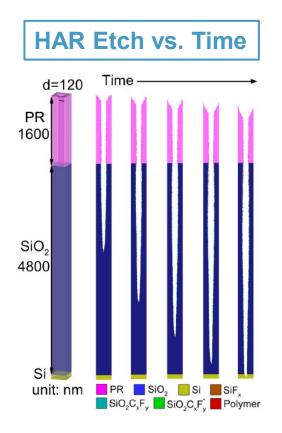
Reactions <sup>e</sup>	Poh	En (eV)	$E_r (eV)^h$	Notes
$SiO_2C_3F_6(s) + I^+ \rightarrow SiO_2CF_3(s) + C_2F_3 + I(h)$	0.75	35	140	Lm
$SiOCF_3(s) + I^+ \rightarrow SiF_3 + CO + I(h)$	0.75	35	140	i,m
$SiO_2CF^*(s) + I^* \rightarrow SiF + CO_2 + I(h)$	0.75	35	140	i,m
$SiO_2CF_2^+(s) + I^+ \rightarrow SiF_2 + CO_2 + I(h)$	0.75	35	140	i,m
$SiO_2CF_3$ *(s) + I* $\rightarrow$ $SiF_3 + CO_2 + I(h)$	0.75	35	140	Lm.
$SiO_2C_2F_3$ *(s) + I* $\rightarrow$ $SiOCF_3$ (s) + CO + I(h)	0.75	35	140	Lm
$SiO_2C_2F_4$ *(s) + I* $\rightarrow$ $SiOCF_3$ (s) + $COF$ + I(h)	0.75	35	140	im.
$SiO_2C_3F_5*(s) + I^* \rightarrow SiO_2CF(s) + C_2F_4 + I(h)$	0.75	35	140	im
$SiO_2C_3F_6$ *(s) + I* $\rightarrow SiO_2CF_3$ (s) + $C_2F_3$ + I(h)	0.75	35	140	Lm.
$SiOCF_3$ *(s) + I* $\rightarrow$ $SiF_3$ + $CO$ + I(h)	0.75	35	140	
Polymer deposition on activated complex				
$SiO_2C_mF_n^+(s) + CF \rightarrow SiO_2C_mF_n^+(s) + P(s)$	0.002 0.0015			
$SiO_2C_mF_n^*(s) + CF_2 \rightarrow SiO_2C_mF_n^*(s) + P(s)$ $SiO_2C_mF_n^*(s) + CF_3 \rightarrow SiO_2C_mF_n^*(s) + P(s)$	0.001			
$SiO_2C_mF_n^*(s) + CF_3 \rightarrow SiO_2C_mF_n^*(s) + P(s)$ $SiO_2C_mF_n^*(s) + C_xF_v \rightarrow SiO_2C_mF_n^*(s) + P(s)$	0.001			k
$SiO_2C_mP_n^{-1}(s) + C_xP_y \rightarrow SiO_2C_mP_n^{-1}(s) + P(s)$ $SiOCF_1^{+}(s) + CF \rightarrow SiOCF_1^{+}(s) + P(s)$	0.002			
$SiOCF_3^*(s) + CF_2 \rightarrow SiOCF_3^*(s) + P(s)$ $SiOCF_3^*(s) + CF_2 \rightarrow SiOCF_3^*(s) + P(s)$	0.002			
$SiOCF_3^*(s) + CF_3 \rightarrow iOCF_3^*(s) + P(s)$	0.001			
SiOCF <sub>1</sub> *(s) + C <sub>2</sub> F <sub>2</sub> $\rightarrow$ SiOCF <sub>3</sub> *(s) + P(s)	0.001			k k
Polymer deposition on polymer	0.001			
$P(s) + CF \rightarrow P(s) + P(s)$	0.002			
$P(s) + CF_2 \rightarrow P(s) + P(s)$	0.0015			
$P(s) + CF_3 \rightarrow (s) + P(s)$	0.001			
$P(s) + C_x F_y \rightarrow P(s) + P(s)$	0.001			k
$P^*(s) + CF \rightarrow P^*(s) + P(s)$	0.02			
$P^n(s) + CF_2 \rightarrow P^n(s) + P(s)$	0.015			
$P^{\phi}(s) + CF_3 \rightarrow P^{\phi}(s) + P(s)$	0.01			
$P^{\theta}(s) + C_x F_y \rightarrow P^{\theta}(s) + P(s)$	0.01			k .
Polymer chemical sputtering				
$P(s) + I^+ \rightarrow I(h) + CF_2$	0.3	30	140	j,a
$P^{+}(s) + I^{+} \rightarrow I(h) + CF_{2}$	0.3	30	140	ja ja m
$P(s) + O^+ \rightarrow COF$	0.2	20	100	
$P(s) + O_2^+ \rightarrow O(h) + COF$	0.2	20	100	-
$P^*(s) + O^* \rightarrow COF$	0.2	20	100	
$P^{\theta}(s) + O_2^+ \rightarrow O(h) + COF$	0.2	20	100	-
Polymer chemical erosion				
$P(s) + F \rightarrow CF_2$	0.001			
$P^n(s) + F \rightarrow CF_2$	0.03			
$P(s) + O \rightarrow COF$	0.5			
$P^{o}(s) + O \rightarrow COF$	0.9			
Fluorination and etching of Si $Si(s) + F \rightarrow SiF(s)$	0.01			
$Si(s) + F \rightarrow SiF(s)$ $SiF(s) + F \rightarrow SiF_2(s)$	0.01			
$SiF_2(s) + F \rightarrow SiF_2(s)$ $SiF_3(s) + F \rightarrow SiF_3(s)$	0.02			
$Si\Gamma_2(s) + \Gamma \rightarrow Si\Gamma_3(s)$ $Si\Gamma_4(s) + \Gamma \rightarrow Si\Gamma_4$	0.05			
Chemical, physical sputtering $Si(s)$ , $SiF_s(s)$	0.00			
Si(s) + $I^+ \rightarrow Si + I(h)$	0.1	37.5	100	Ref. 40,13
$SiF(s)+I^+ \rightarrow SiF+I(h)$	0.3	10	100	im.
$SiF_2(s) + I^+ \rightarrow SiF_2 + I(h)$	0.4	10	100	i,m
$SiF_3(s) + I^+ \rightarrow SiF_3 + I(h)$	0.5	10	100	Lm
Polymer deposition on Si(s) and SiF <sub>s</sub> (s)				
$Si(s) + CF \rightarrow Si(s) + P(s)$	0.5			
$Si(s) + CF_2 \rightarrow Si(s) + P(s)$	0,375			
$Si(s) + CF_3 \rightarrow Si(s) + P(s)$	0.25			
$Si(s) + C_xF_y \rightarrow Si(s) + P(s)$	0.25			k .
$SiF_x(s) + CF \rightarrow SiF_x(s) + P(s)$	0.002			
$SiF_x(s) + CF_2 \rightarrow SiF_x(s) + P(s)$	0.0015			
$SiF_x(s) + CF_3 \rightarrow SiF_x(s) + P(s)$	0.001			
$SiF(e) + C F \rightarrow SiF(e) + P(e)$	0.001			k

Reactions	$p_0$	$E_{th} (eV)^h$	$E_r (eV)^b$	Notes
Redeposition of SiF <sub>x</sub>				
$P(s) + SiF_x \rightarrow P(s) + SiF_x(s)$	0.001			
Erosion of photoresist				
$R(s) + I^+ \rightarrow R + I(h)$	0.01	20	100	4
$R(s) + O \rightarrow COH$	10 <sup>-5</sup>			
Redeposition of gas phase photoresist				
$W(s) + R \rightarrow W(s) + R(s)$	0.01			
Polymer deposition on photoresist				
$R(s) + CF \rightarrow R(s) + P(s)$	0.02			
$R(s) + CF_2 \rightarrow R(s) + P(s)$	0.015			
$R(s) + CF_3 \rightarrow R(s) + P(s)$	0.01			
$R(s) + C_xF_y \rightarrow R(s) + P(s)$	0.01			, k
	$p_0^p$	<i>E</i> <sub>sh</sub> (eV) <sup>p</sup>	$E_m$ (eV) <sup>p</sup>	Notes
Activation by low energy ions				
$SiO_2C_mF_n(s) + I^+ \rightarrow SiO_2C_mF_n^+(s) + I(h)$	0.1	5	70	- 4
$SiOCF_3(s) + I^+ \rightarrow SiOCF_3*(s) + I(h)$	0.1	5	70	- 4
$P(s) + M^+ \rightarrow P^*(s) + M(h)$	0.3	5	30	44
Polymer deposition by low energy ions				
$SiO_2C_mF_n(s) + CF_x^+ \rightarrow SiO_2C_mF_n(s) + P(s)$	0.1	5	70	j,k
$SiO_2C_mF_n(s) + C_xF_y^+ \rightarrow SiO_2C_mF_n(s) + P(s)$	0.1	5	70	j,k
$SiOCF_3(s) + CF_x^+ \rightarrow SiOCF_3(s) + P(s)$	0.1	5	70	j.k
$SiOCF_1(s) + C_sF_{s'}^+ \rightarrow SiOCF_2(s) + P(s)$	0.1	5	70	18

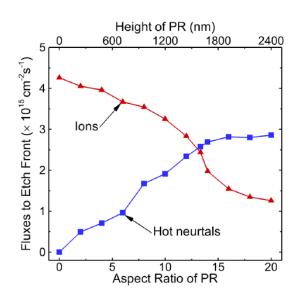


## **Huang – HAR Dielectric Etch – Feature Scale Results**

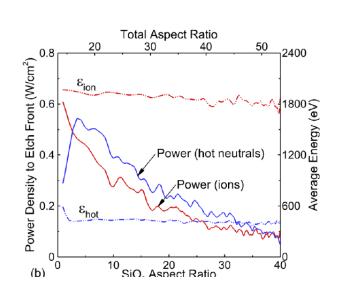
- Simulations were used to understand how the etch process evolves with increasing aspect ratio (AR).
- lons converted to "hot neutrals" when they impacted the sidewalls inside trenches.
- Power delivered to the feature bottom decreased with AR due to increased energy loss on sidewall impact.
- They demonstrated how the profile can be controlled by changing the ratio of  $C_xF_v$  neutrals to ions.

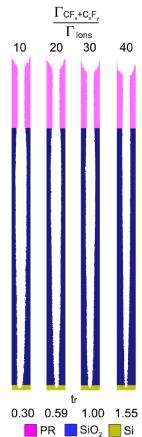






## Power vs. Aspect Ratio





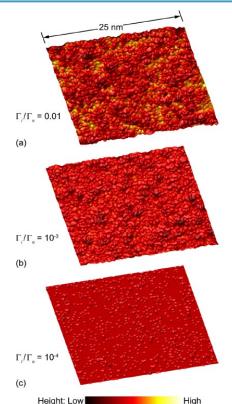




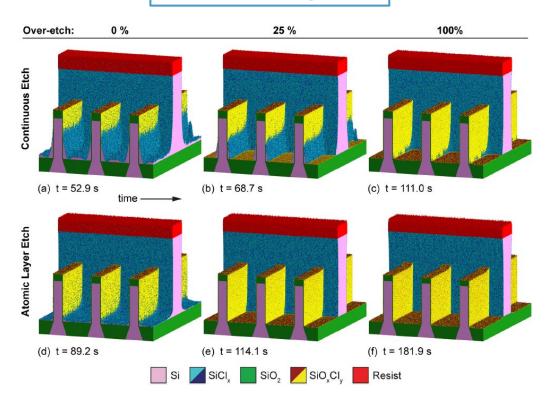
## Huard – Si Atomic Layer Etch (ALE) – Feature Scale Results

- Huard et al. used the same codes (HPEM+MCFPM) to investigate Si ALE under non-ideal conditions.
- The found that high neutral / ion flux ratio is needed to get smooth surface during ALE.
- ALE during over-etching helps get clean fin profiles in less time with reduced damage.

## Surface Roughness vs. $\Gamma_i/\Gamma_n$



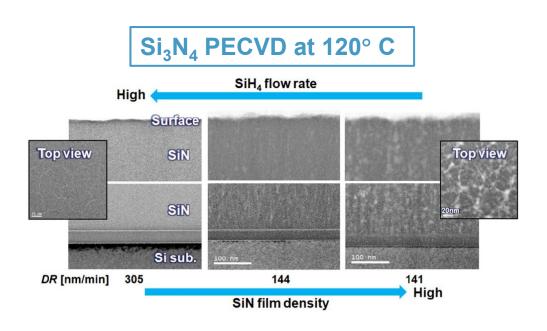
## **Profile During Etch**





#### Kuboi – PECVD Feature Scale Model

- Kuboi *et al.* studied plasma enhanced CVD deposition of Si<sub>3</sub>N<sub>4</sub> in SiH<sub>4</sub>/NH<sub>3</sub>/N<sub>2</sub> and SiH<sub>4</sub>/N<sub>2</sub>O.
- Experiments showed that, when deposited at 120° C, the film is columnar at low flow rate.
- Modeling was done using a Monte Carlo feature scale model that included surface migration.



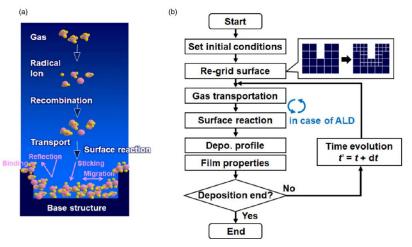


Fig. 2. (Color online) (a) Schematic of the deposition process and (b) calculation flow chart of the 3D deposition model.

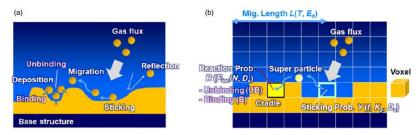
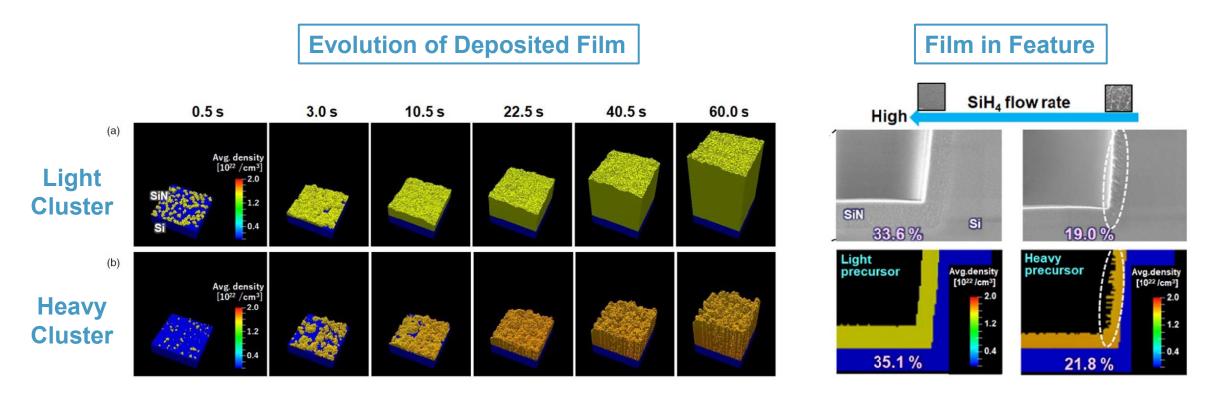


Fig. 3. (Color online) Schematic pictures of (a) actual phenomena on the deposited surface over the base structure: irradiation of gas, sticking, reflection, migration, and binding and (b) corresponding deposition model using a statistical ensemble method in the voxel space



## Kuboi – PECVD Feature Scale Model

- The structure of the film vs. SiH₄ flow was attributed to recombination in gas phase.
- Longer residence time at lower SiH<sub>4</sub> flow led to formation of larger clusters in the gas, producing columnar film growth.

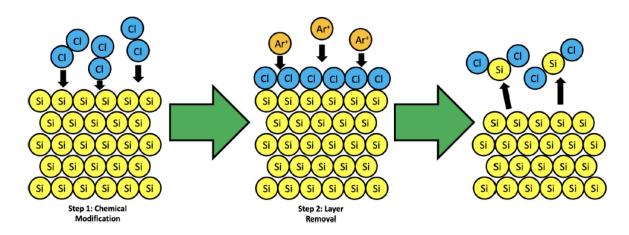




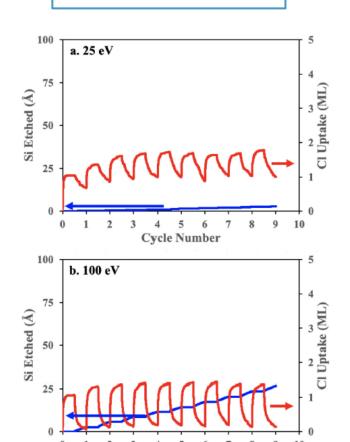
## Vella – Si Atomic Layer Etch (ALE) – Molecular Dynamics (MD) Model

- Vella and Graves used a MD model to examine Si ALE in Cl<sub>2</sub> + Ar plasma.
- They used the REBO potential developed earlier in their group to model the Si-Cl system.
- Etch is self-limiting and close to ideal ALE at 25 eV. The etch rate is low.
- With increasing ion energy, etching does not stop during the etch step.

#### Ideal Si-Cl<sub>2</sub>-Ar Atomic Layer Etch Process



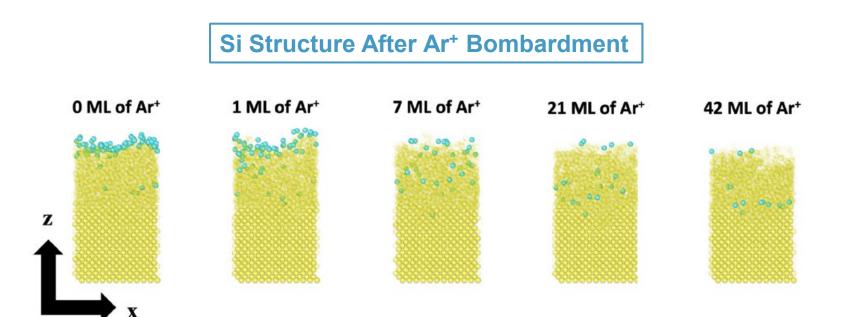
#### Si Etched vs. Time



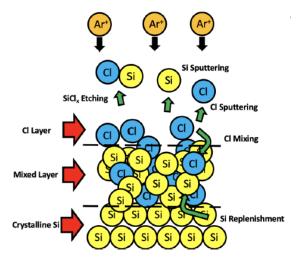


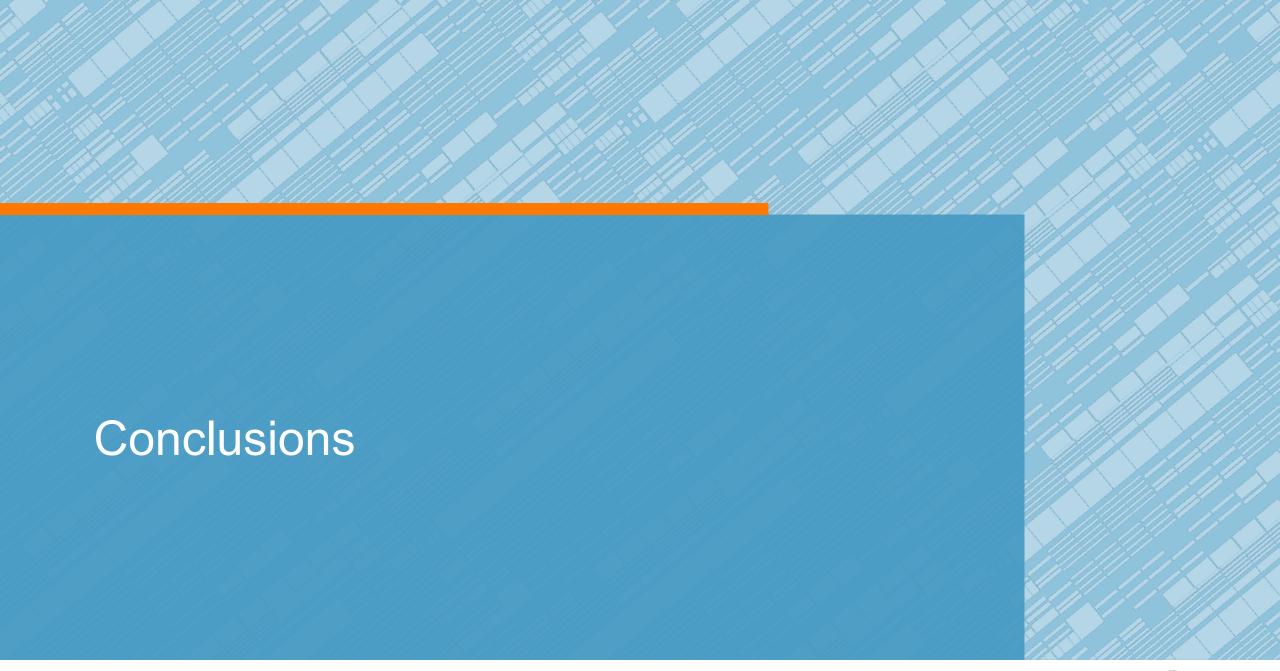
#### Vella - Si ALE - MD Results

- It was shown that if multiple ions are used during the ion bombardment step, the structure seen by the ion changes with time. The last ions experience a more physical sputtering like condition.
- Ions create a mixed layer near the surface with some residual CI.



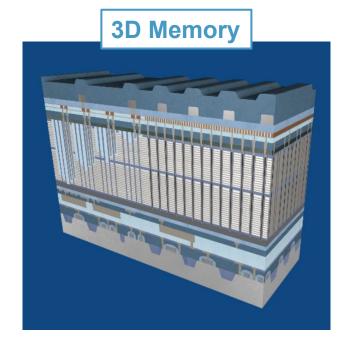
## What's Happening Near the Surface?



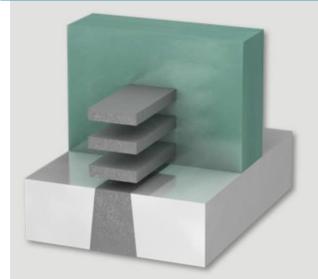


## The Future of Plasma and Feature Scale Modeling

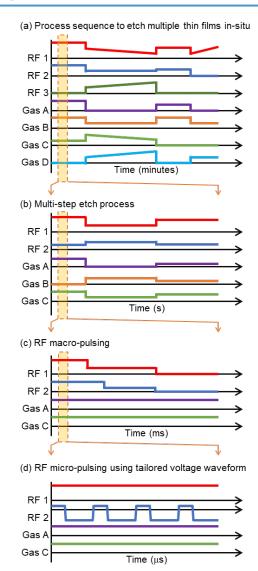
- Complexity of microelectronics technologies increasing immensely:
  - ▶ 3D architectures
  - nm-sized features
  - ▶ Atomic level precision during manufacturing on 300 mm wafers
- Precise control of every aspect of the plasma required.
- Resulting complexity making modeling ever more critical for advancing plasma technology.



## Gate All Around Transistor



## **Typical Plasma Etch Process**





#### Conclusions

- Low T<sub>e</sub> plasmas are a vital technology used for microelectronics manufacturing.
- Plasma modeling plays active role in plasma technology development in industry.
- Semiconductor industry is one of the largest employer of plasma modeling engineers.
- Plasma modeling engineers in industry:
  - Actively participate in R&D, product design, and customer communication
  - Use a variety of specialized software tools
  - Work on a diverse set of technically challenging problems
  - Need strong foundation in plasma physics and plasma surface interactions to be successful
- Examples were used to illustrate the types of modeling work done in industry.
- Close connection to experiments and focus on solving major technological problems are key.



