

Introduction to Plasma Physics and Plasma Processes

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Ho Jun Kim
Assistant Professor

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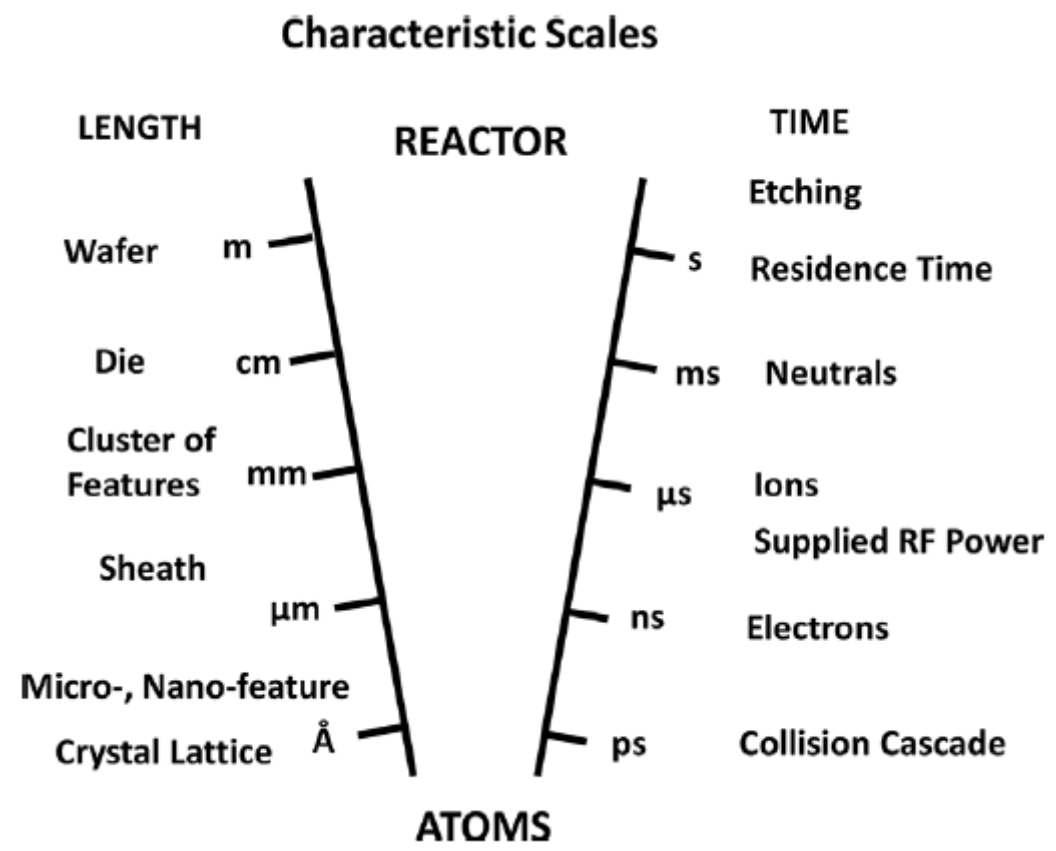
EDUCATION

- Ph.D.** Texas A&M University,
College Station, Texas, 2008
Major: Mechanical Engineering
- M.S.** Texas A&M University,
College Station, Texas, 2004
Major: Mechanical Engineering
- B.S.** Hanyang University,
Seoul, South Korea, 2002
Major: Mechanical Engineering



EXPERIENCE

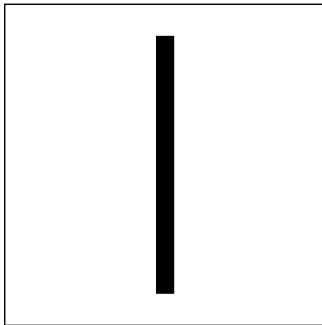
- Assistant Professor** Dong-A University, Department of Mechanical Engineering.
(3/18 – *)
- Principal Engineer** Samsung Electronics, Memory Thin Film Technology Team.
(3/14 – 2/18)
- Senior Engineer** Samsung Electronics, Memory Thin Film Technology Team.
(8/08 – 2/14)
- Research Expert** Korea Institute of Industrial Technology, Fuel Cell Group.
(3/08 – 7/08)
- Research Associate** Old Dominion University, Department of Mechanical and Aerospace Engineering.
(1/07 – 2/08)
- Research Assistant** Texas A&M University, Department of Mechanical Engineering. (9/03 – 12/06)



Complex Flows and Plasma Physics Laboratory (CFPPL)

Chaotic Transport

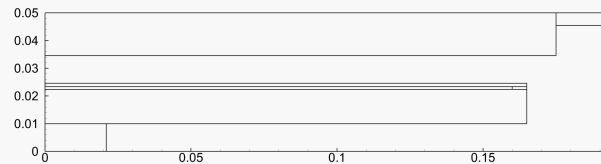
- Computation of stretching and its efficiency in chaotic flows
- Mixing, reaction and chaos in multi-dimensional flows
- Periodic point and invariant manifold in chaotic flows



Chaotic cavity flow

Plasma Discharge

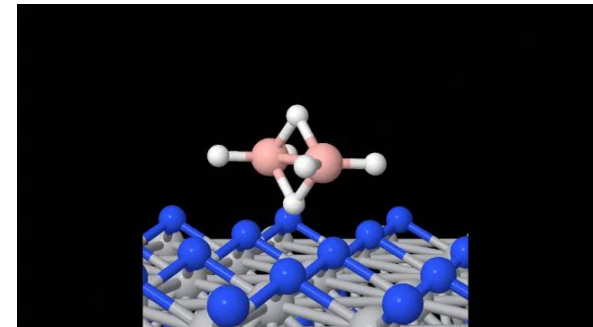
- Process plasma (CCP) simulations: PE-TEOS, PE-SiN, PE-SiON, ACL, PE-ALD
- Process plasma (ICP) simulations: HDP-SiO₂, HDP-SiN, HDP-ACL
- Remote plasma: fluorine chemistry, NF₃ plasma dissociation, fluorine transport



Electron density

Surface Chemistry

- Molecular dynamics: deposition, etching
- Ab initio calculation: reaction rate, activation energy
- Computational chemistry: reaction rate, reaction pathway

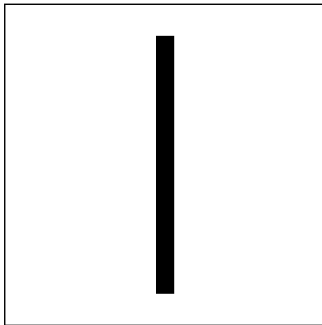


Dissociation reaction of B₂H₆ on TiN surfaces

Complex Flows and Plasma Physics Laboratory (CFPPL)

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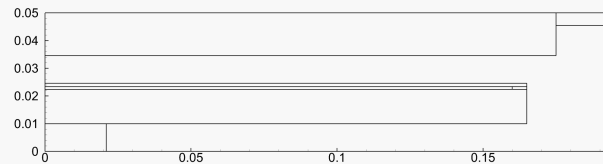
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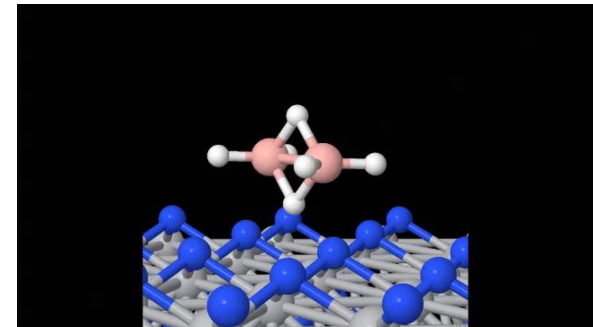
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Surface Chemistry

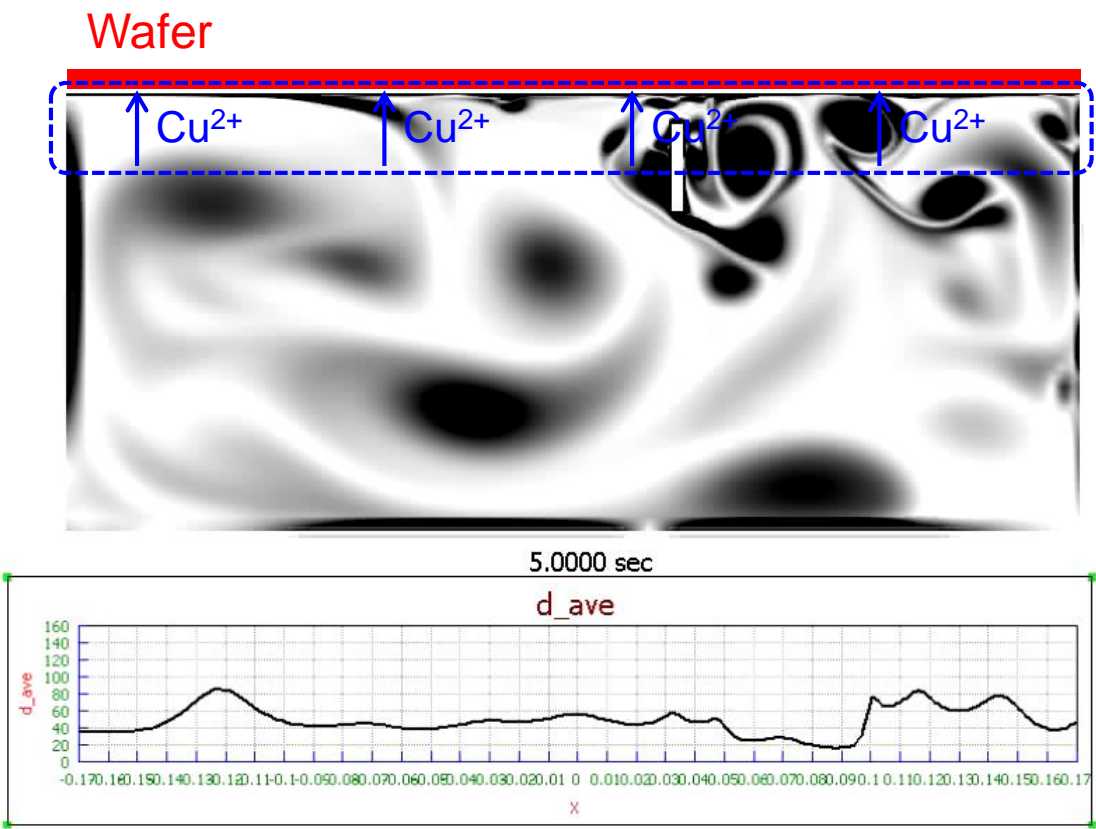
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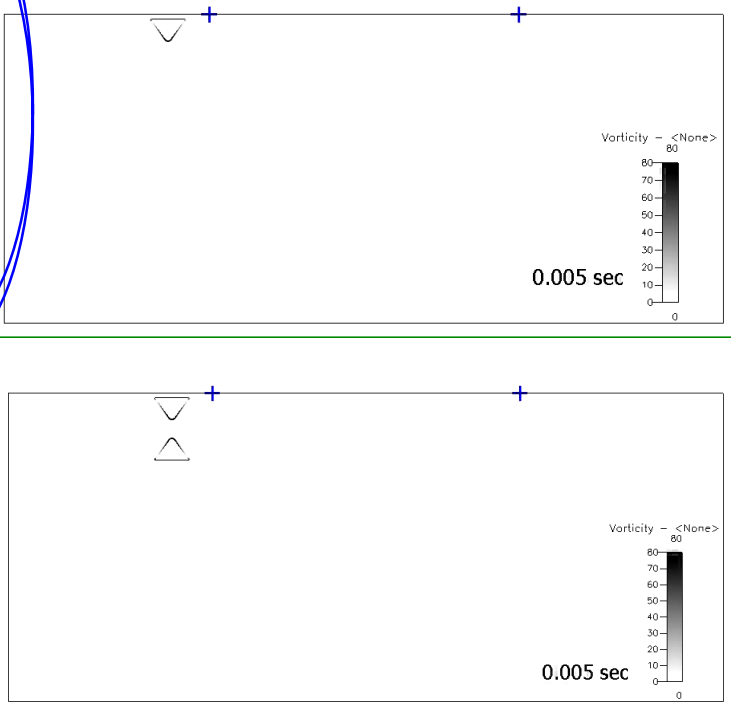
Dissociation reaction of B₂H₆ on TiN surfaces

Process simulation: Electroplating of Cu

Active type (moving stirrer) reactor: vortex contour

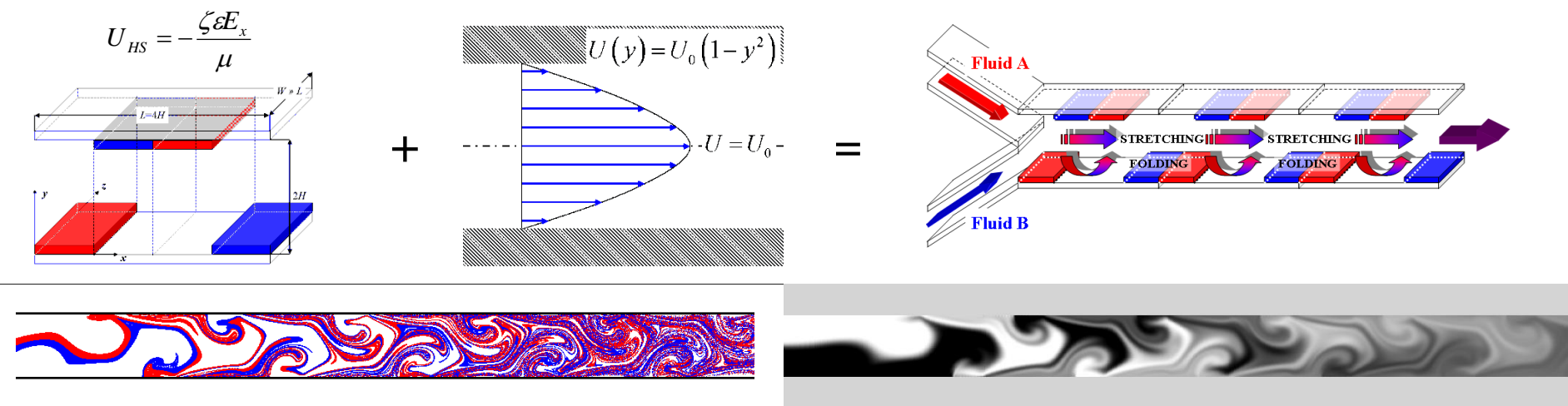


By the vortex movement, the surface flux of Cu ion is uniformly formed along the wafer surface.



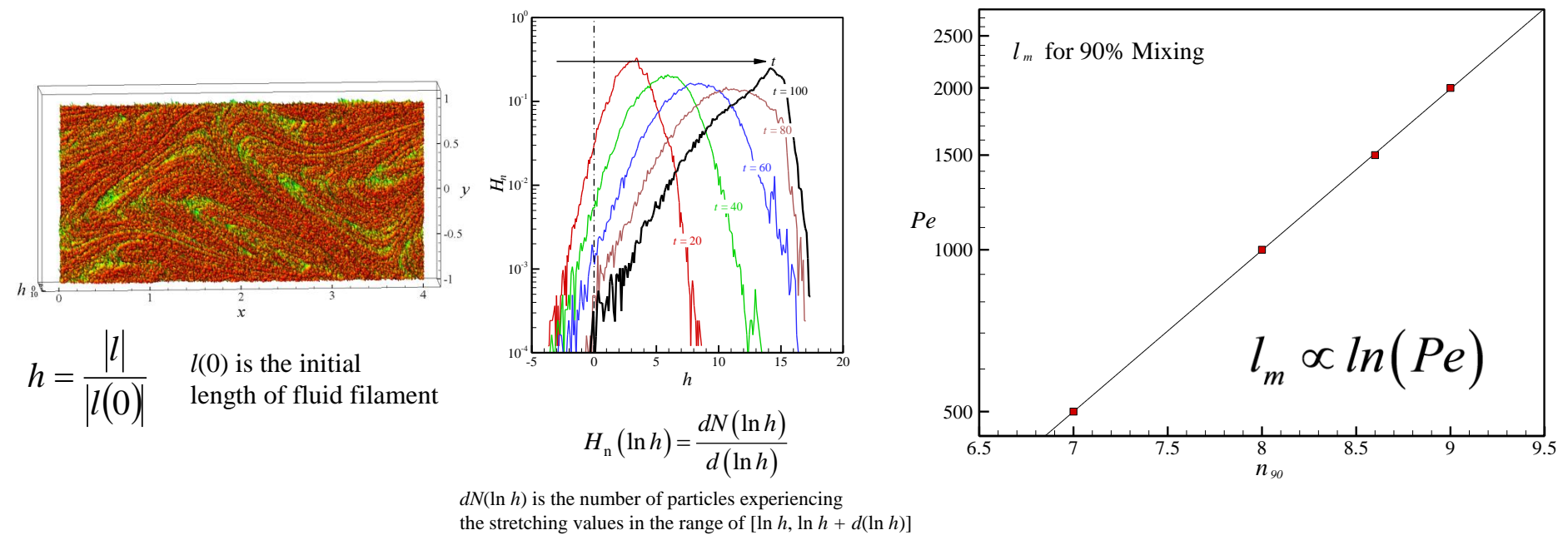
Examples of stirrer design

Electroosmotically stirred chaotic micro mixer



Particle Dispersion

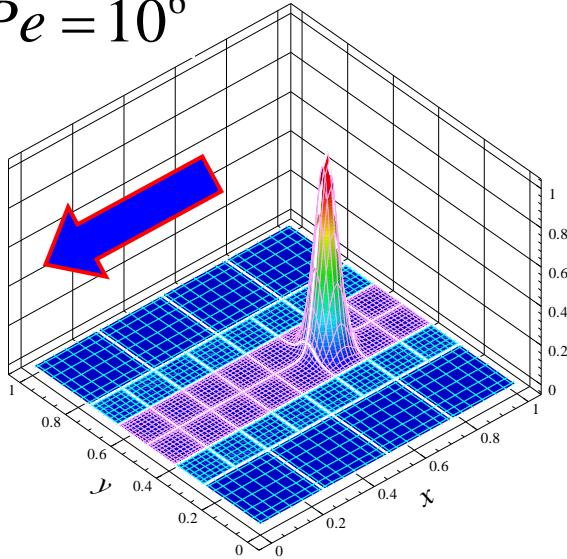
Mixing Simulation, $Pe = 1000$



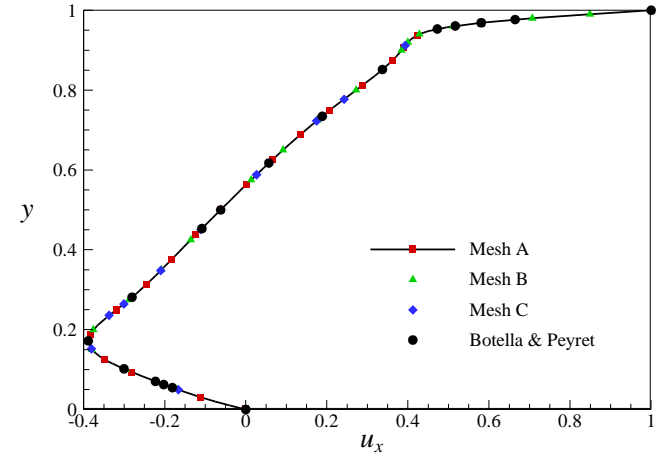
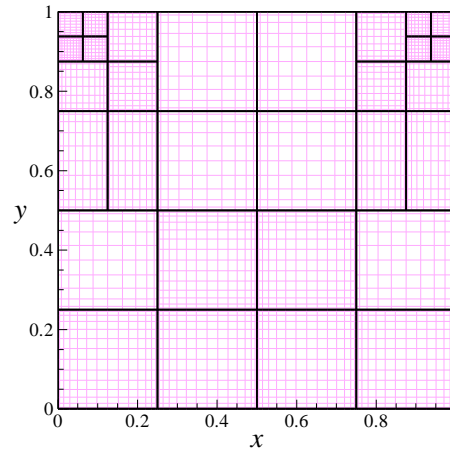
Nonconforming spectral element method

Moving Gaussian Hill

$Pe = 10^6$



Singular cavity flow, $Re = 1,000$



u_x velocity distribution along the $x = 0.5$ line

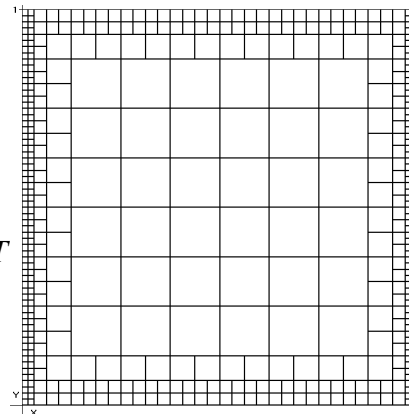
Boussinesq approximation: Natural convection

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0$$

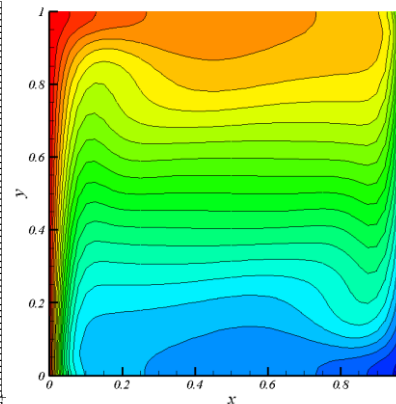
$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = -\frac{\partial p}{\partial x} + \frac{Pr}{Ra^{1/2}} \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right)$$

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} = -\frac{\partial p}{\partial y} + \frac{Pr}{Ra^{1/2}} \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) + PrT$$

$$\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} = \frac{1}{Ra^{1/2}} \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right)$$

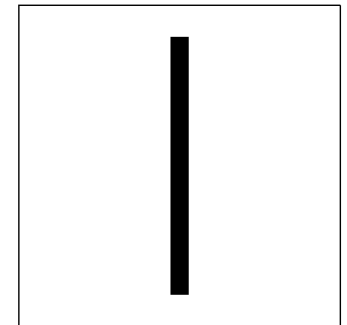


mesh



temperature

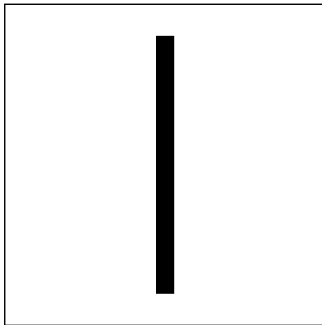
Chaotic flow in a cavity



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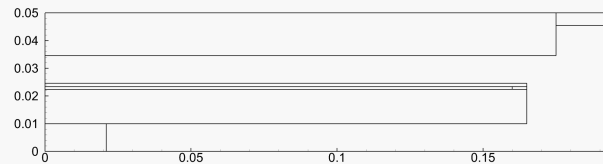
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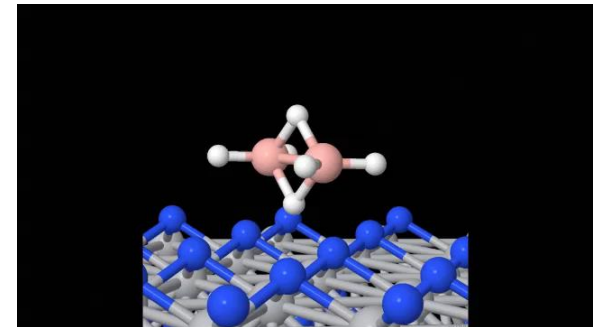
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Electron density

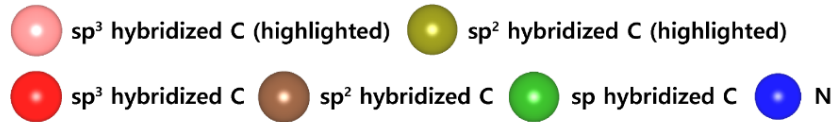
Surface Chemistry

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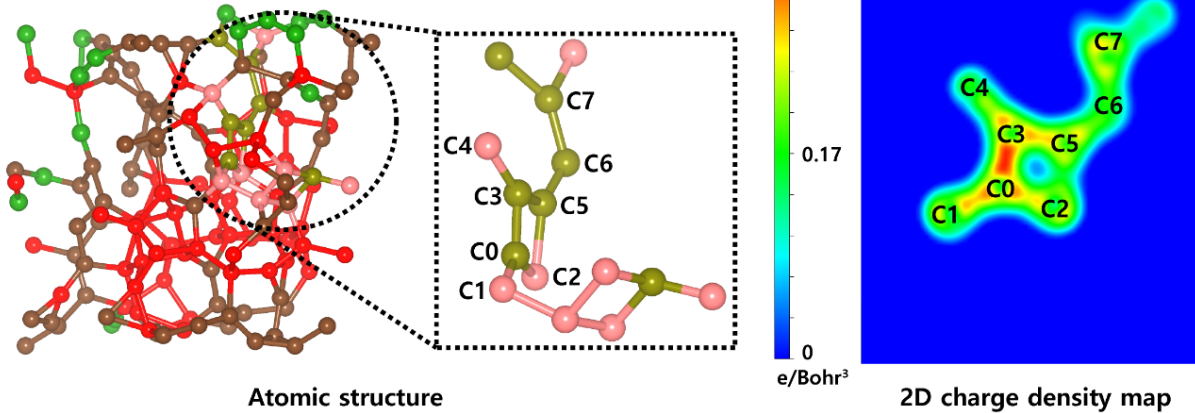


Dissociation reaction of B₂H₆ on TiN surfaces

The optimized structures of ACL and 2D charge density map



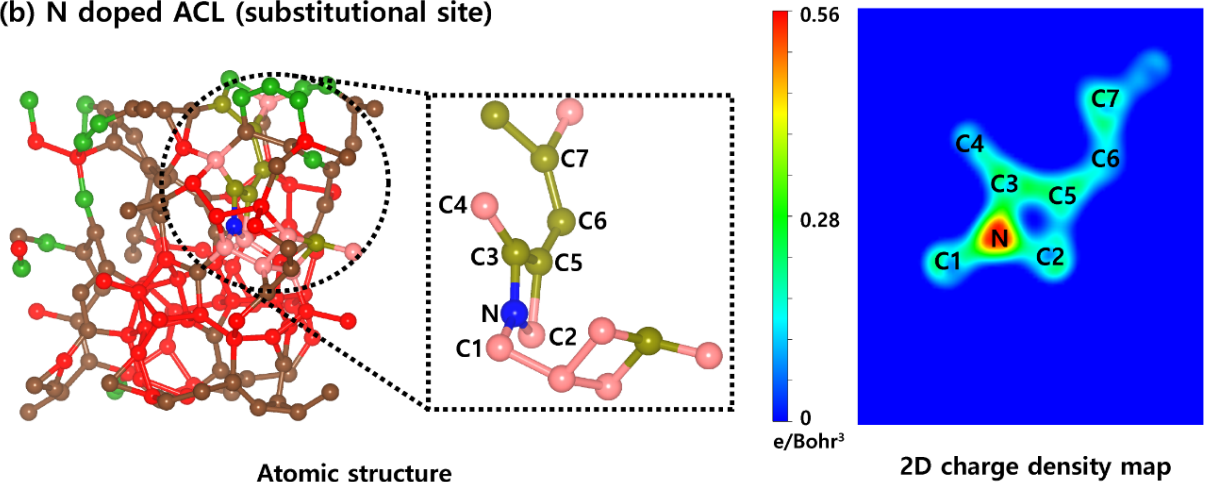
(a) Undoped ACL



The optimized structures of the ACL (left) and 2D charge density map (right) for (a) undoped ACL and (b) N doped ACL (substitutional site).

In the center of (a-b), several atoms in the dotted black box are highlighted.

(b) N doped ACL (substitutional site)

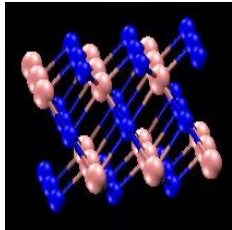


2D charge density map contains specified atoms: (a) C0 ~ C7, and (b) N and C1 ~ C7. Charge accumulation (red area) in the vicinity of the N atom can be seen.

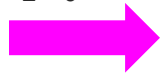
Surface phenomena: Molecule dissociation and deposition

Ab initio simulations

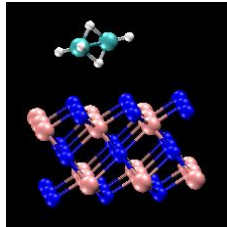
Bare N ter-TiN (111)



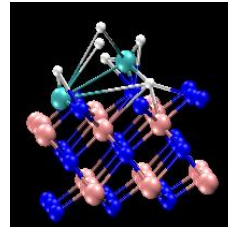
B_2H_6 flow



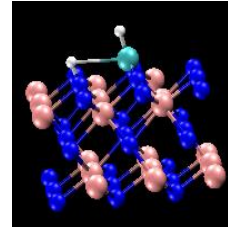
B_2H_6



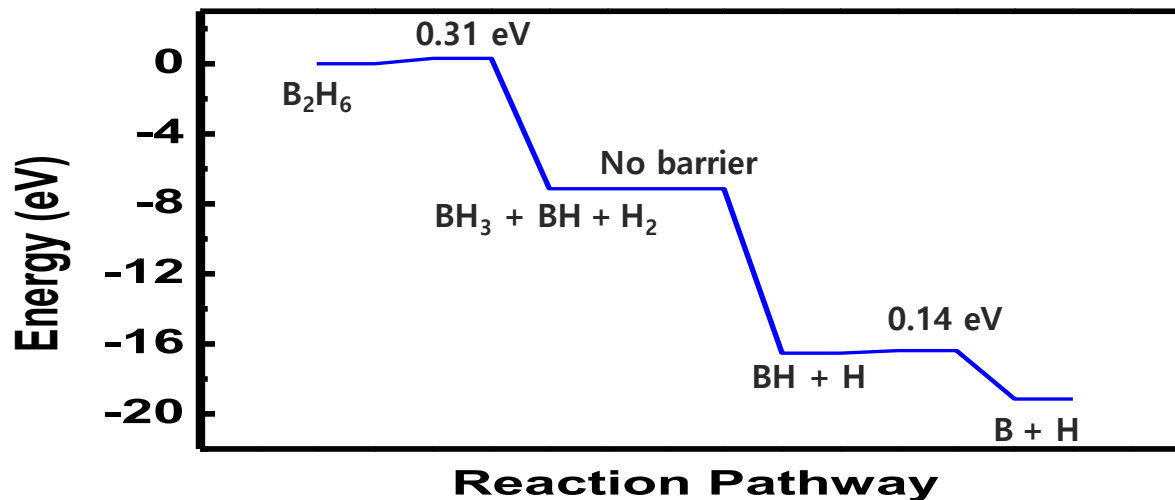
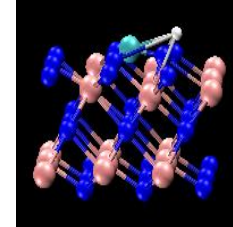
$BH_2 + BH + H + H_2$



$BH + H$



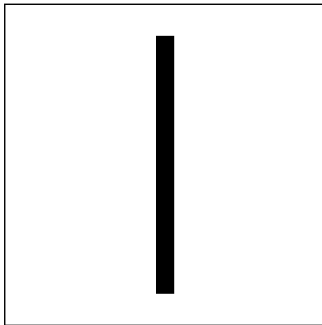
$B + H$



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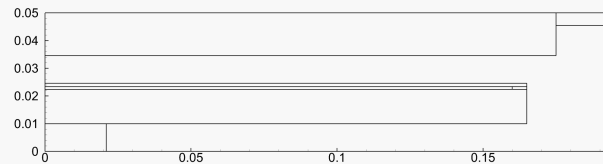
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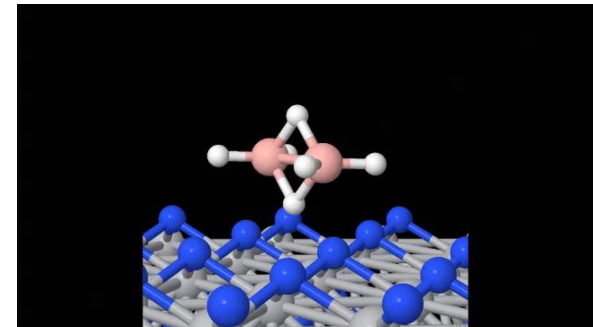
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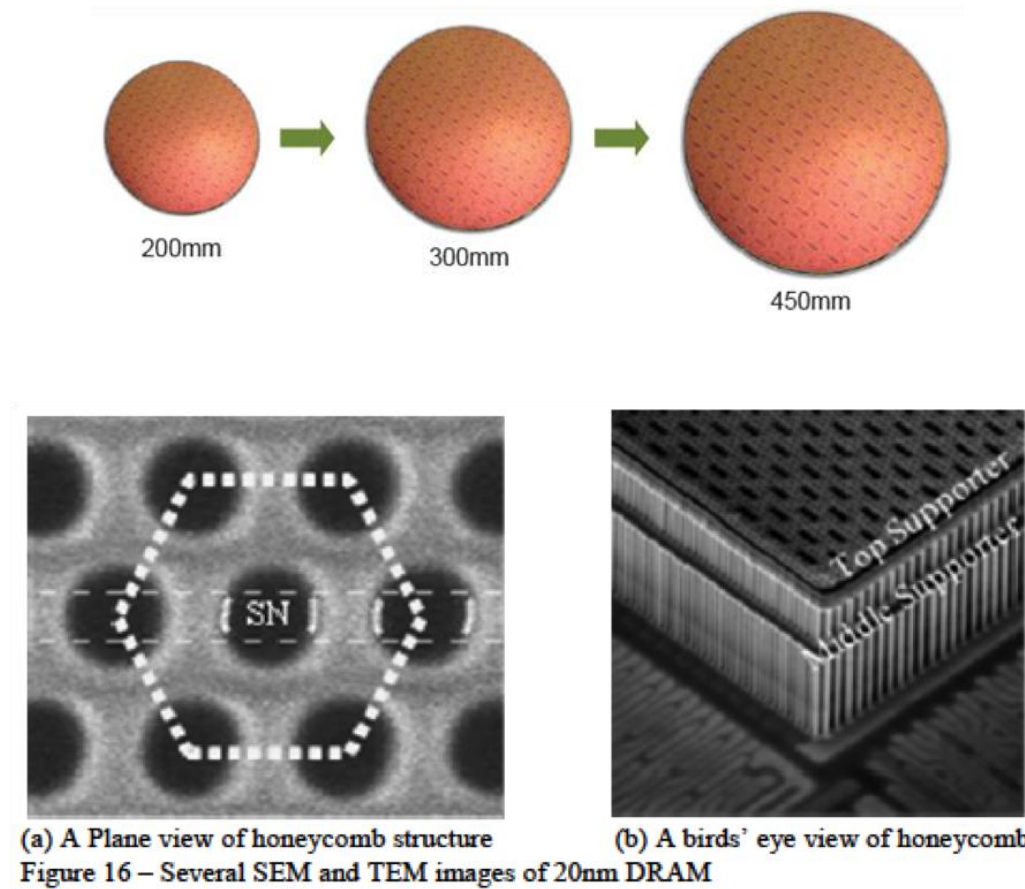
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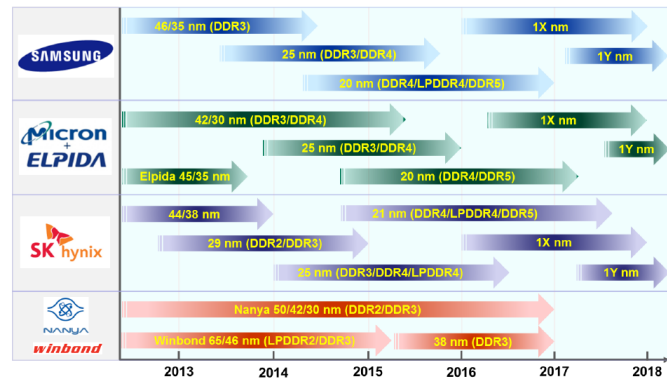
Recent trend in a semiconductor industry



DRAM Technology Review

TECHINSIGHTS

■ DRAM Process Node Roadmap (Manufacturers)



Proposed 3D NAND Structure

	p-BiCS (Toshiba)	TCAT (Samsung)	3D FG (Hynix)	Micron
Structure				
Key Features	- P+ SONOS Cell	- TANOS Cell	- Floating Gate	?
Key Issue	- Large Cell Size - Reliability	- Large Cell Size - SL Resistance	- Process of bit separation - Disturbance	?

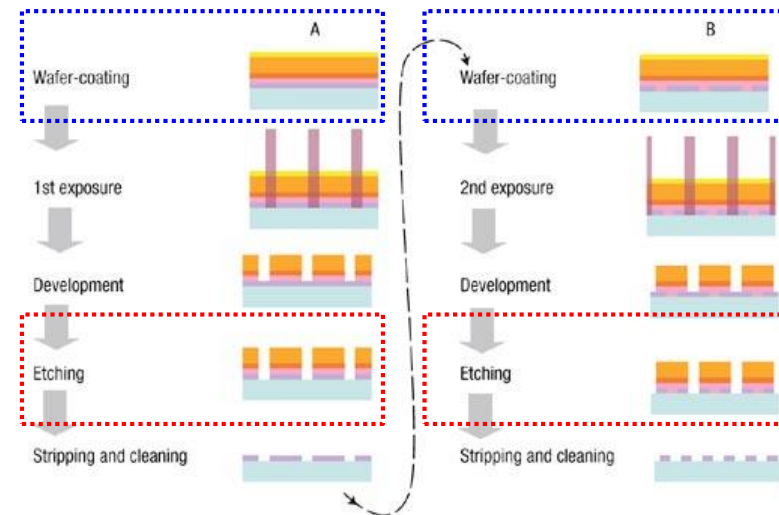
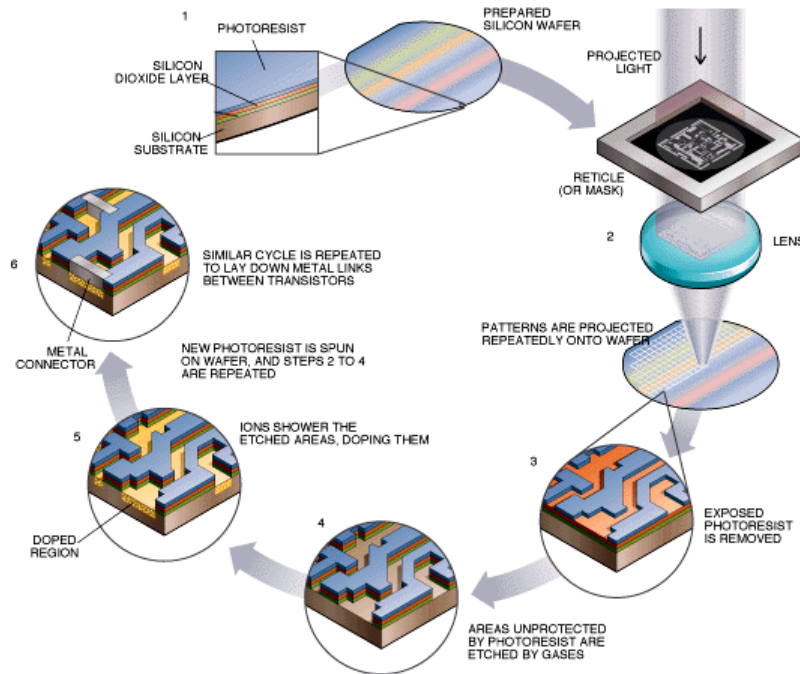
Source: TechInsights

Semiconductor fabrication process

Semiconductor fabrication consists of the various (total 8) categories of process:

- Photolithography
- Wet Chemical Etching
- Dry Etching
- Diffusion
- Ion Implantation
- Film Deposition – Metallization
- Film Deposition – Dielectric
- Chemical Mechanical Polishing

Plasma is mainly adopted.



> 50 %, plasma process



Samsung Electronics SCS Engineers

Definition of plasma

Plasmas

A collection of freely moving charged particles which is, on the average, electrically neutral

- Discharges:

Driven by voltage or current sources

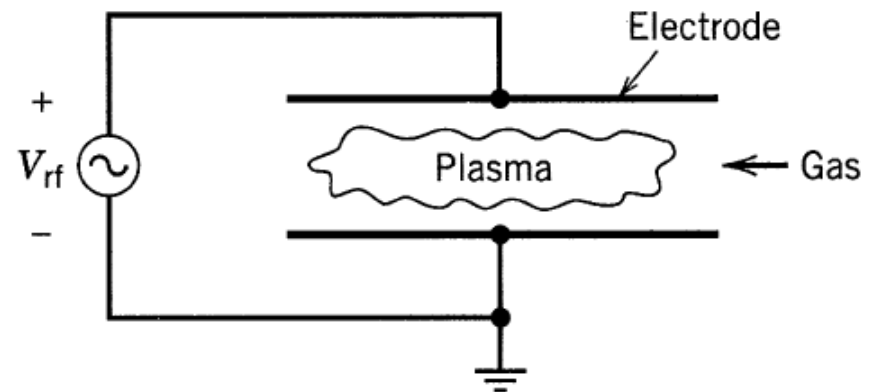
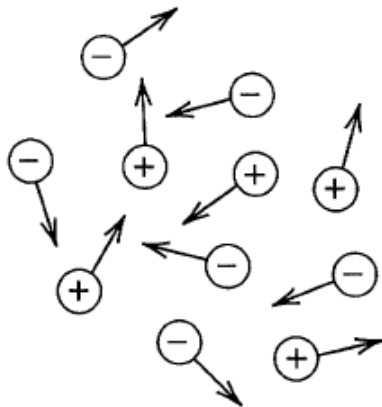
Neutral particles are important

There are boundaries at which surface losses are important

The electrons are much hotter than the ions

- Device sizes: 30 cm - 1 m

- Driving frequencies: DC to RF (13.56 MHz) to microwaves (2.45 GHz)

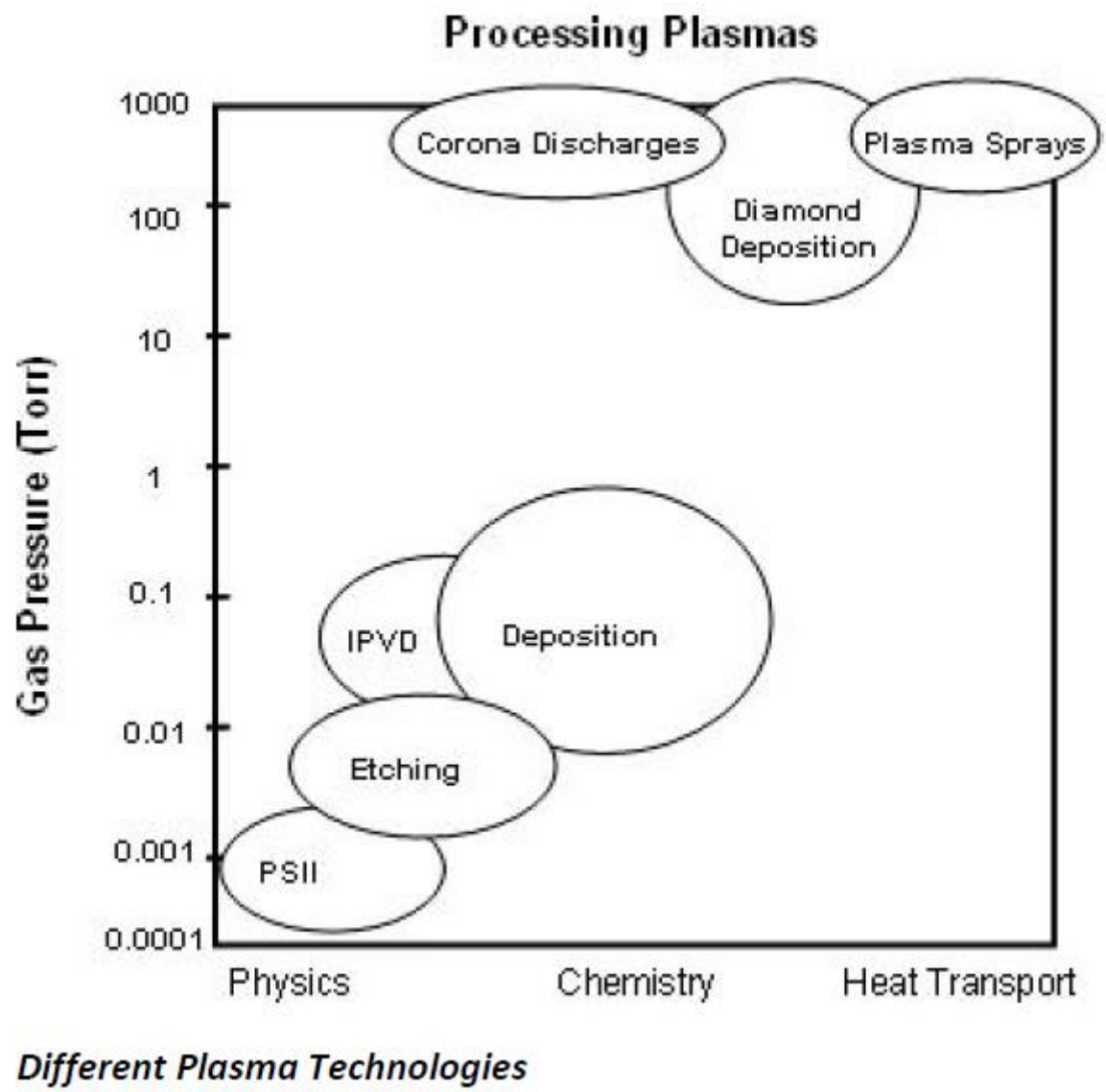


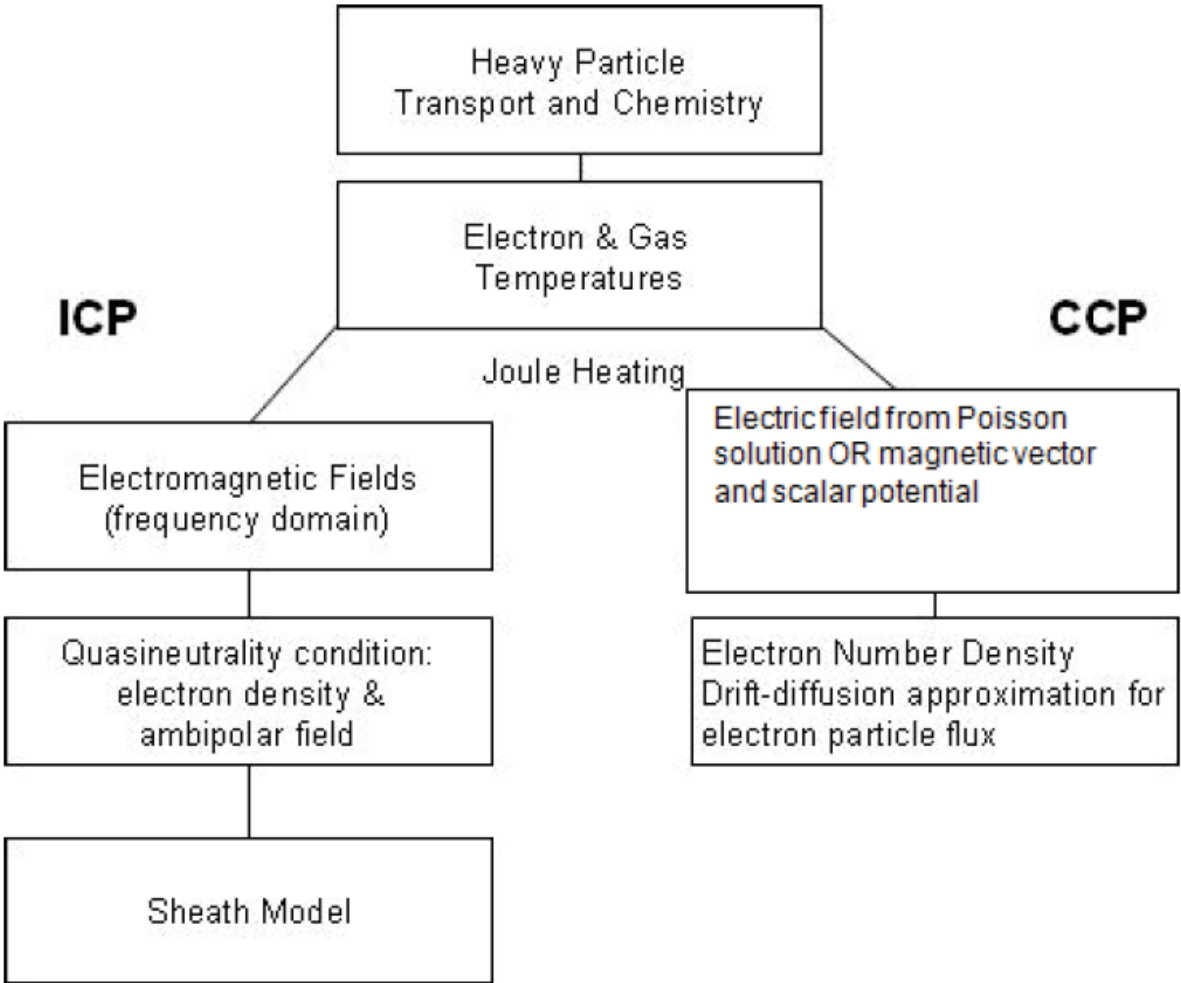
What is
Plasma ?

Plasma: A plasma is a hot ionized gas consisting of approximately equal numbers of positively charged ions and negatively charged electrons. The characteristics of plasmas are significantly different from those of ordinary neutral gases so that plasmas are considered a distinct “fourth state of matter.” For example, because plasmas are made up of electrically charged particles, they are strongly influenced by electric and magnetic fields (see figure) while neutral gases are not. An example of such influence is the trapping of energetic charged particles along geomagnetic field lines to form the Van Allen radiation belts.

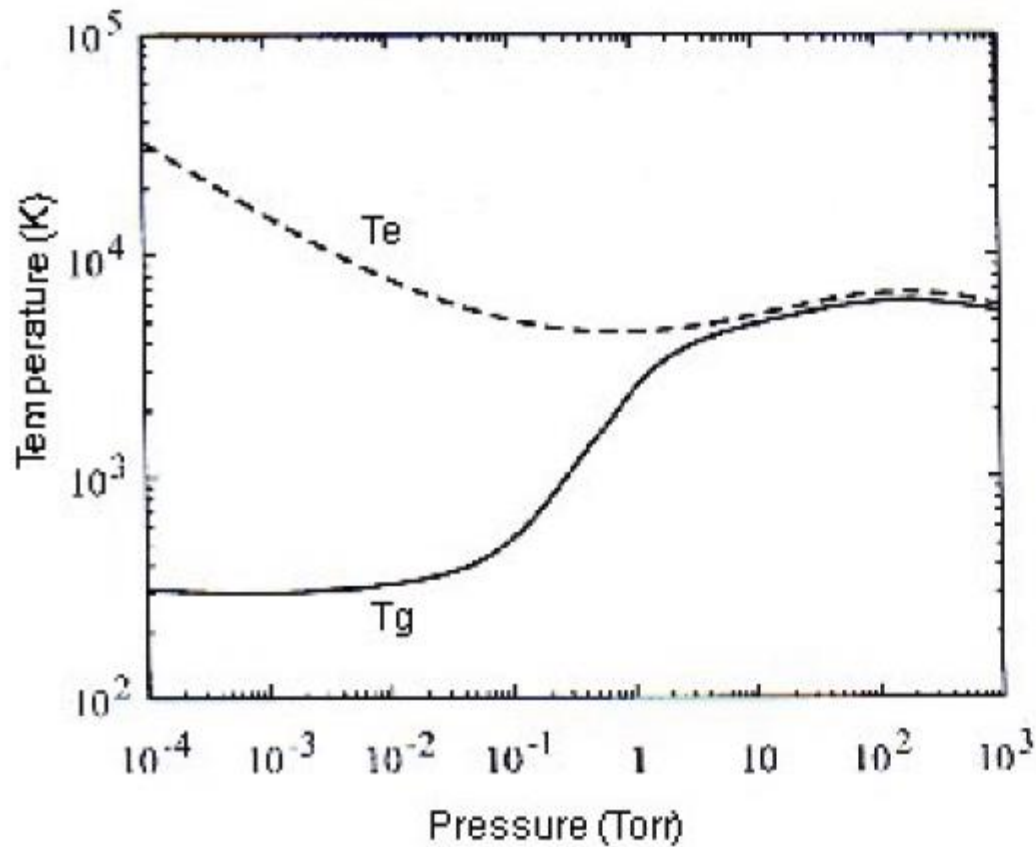


www.geo.mtu.edu/weather/aurora/





Distinctive Features of the ICP and CCP Models



Electron and gas temperatures in a DC discharge of mercury and rare gas mixture at different gas pressures and same current.

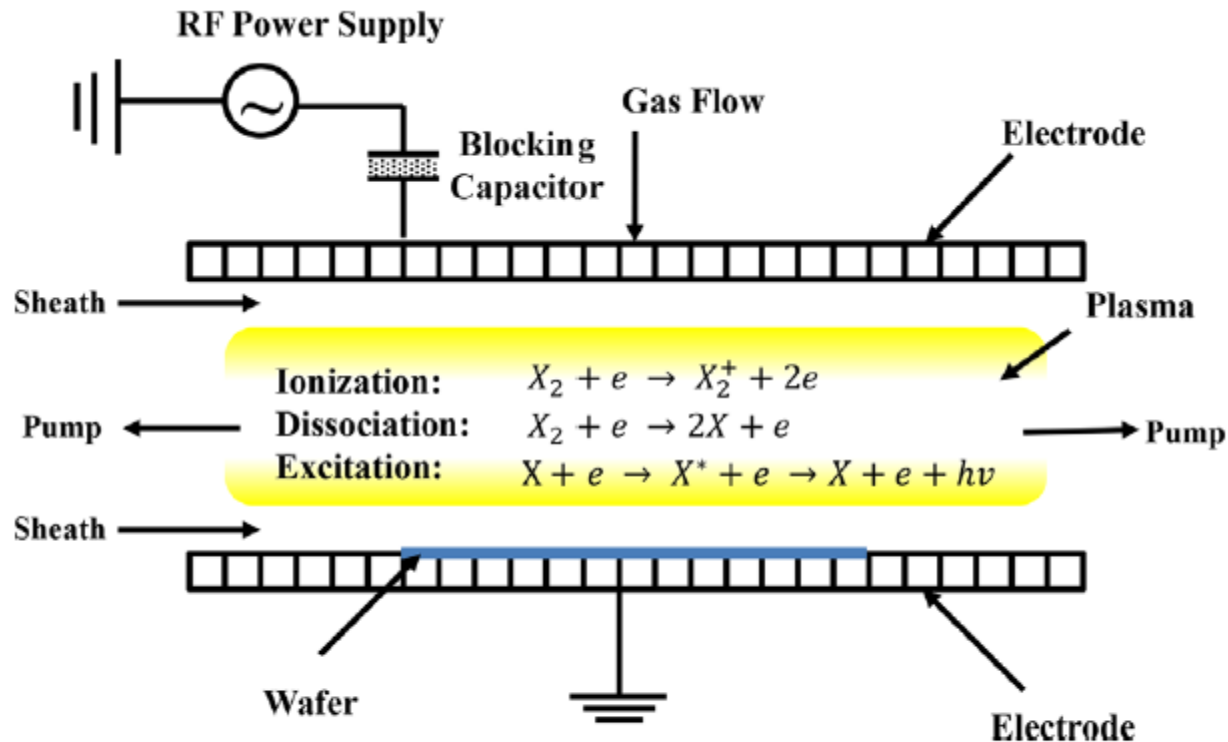


Figure 3. Schematic of a parallel plate capacitively-coupled plasma (CCP) reactor.

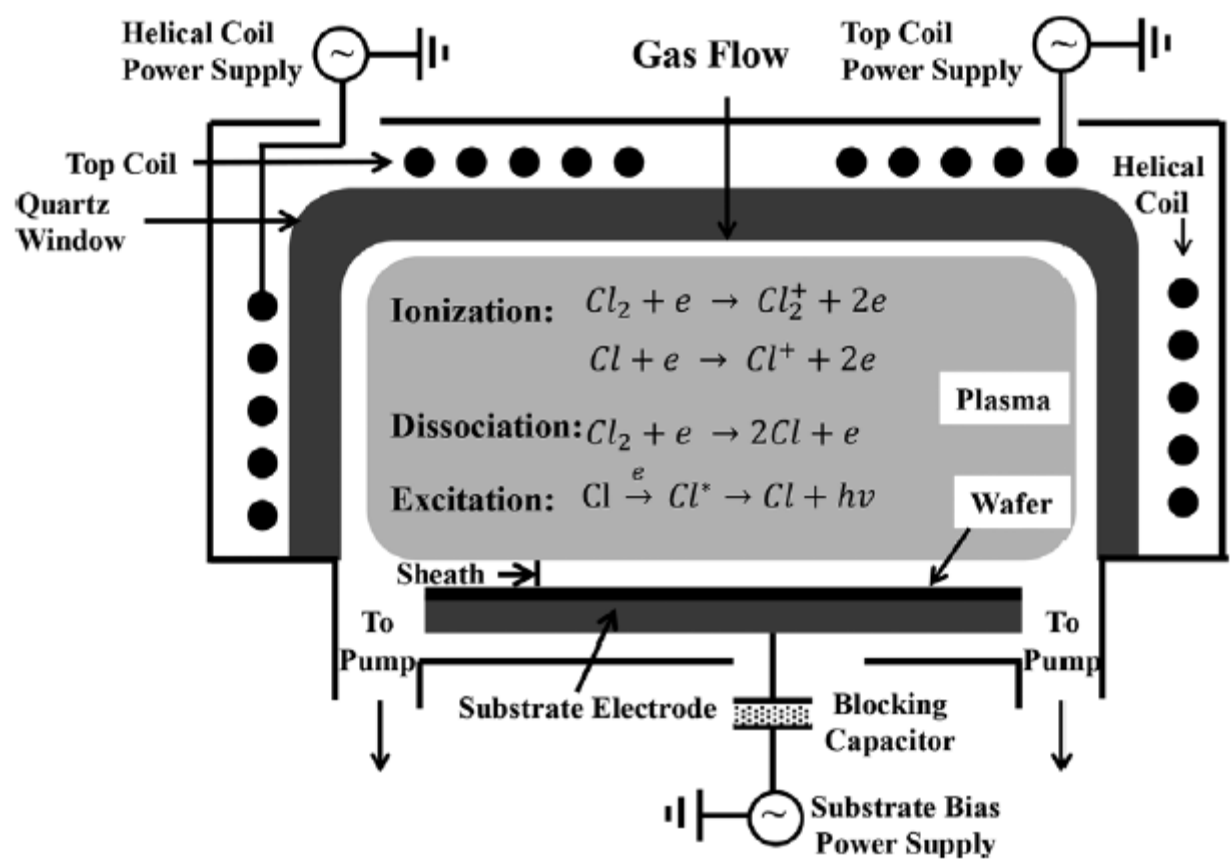


Figure 4. Schematic of a dual coil inductively-coupled plasma (ICP) reactor.

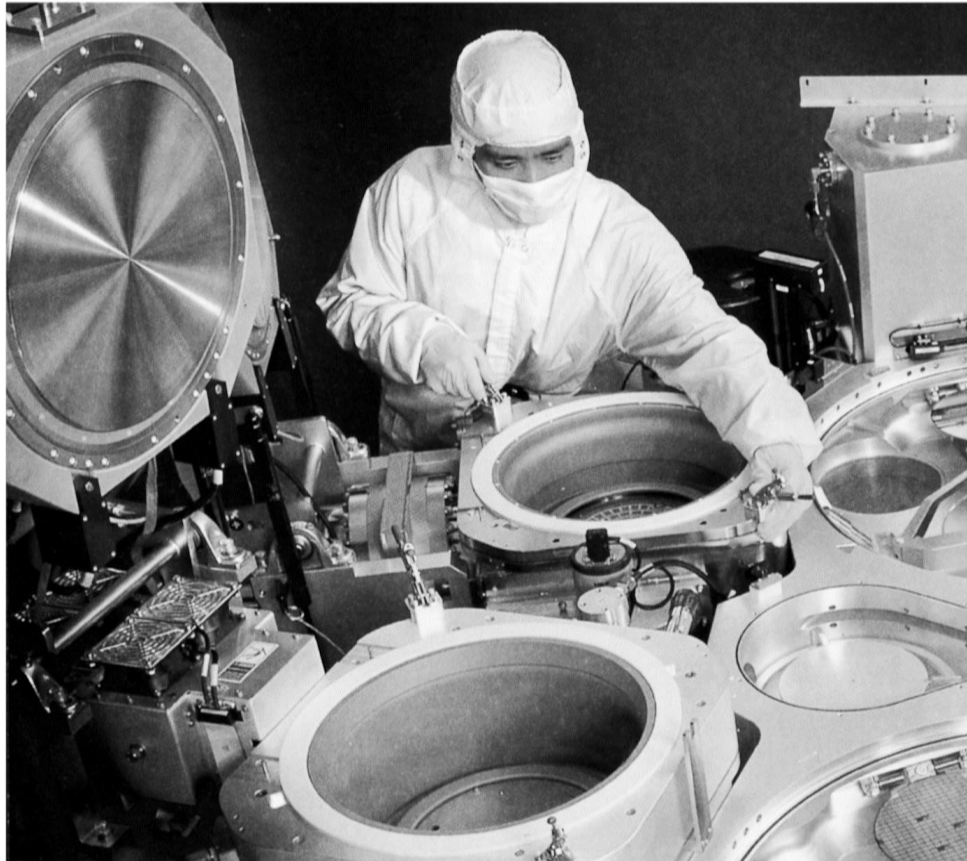


Figure 12.24 The Endura system by Applied Materials uses a number of PVD or CVD chambers fed by a central robot. For conventional and IMP sputtering, targets are hinged to open upward. Two open chambers are shown in this photograph along with the load lock (*from Applied Materials*).

Introduction to Plasma Physics

PLASMAS AND DISCHARGES

- **Plasmas**

A collection of freely moving charged particles which is, on the average, electrically neutral

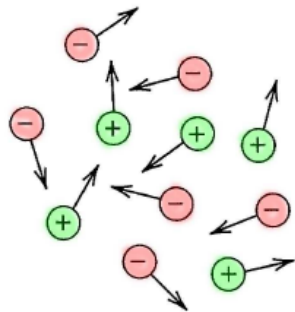
- **Discharges**

Are driven by voltage or current sources

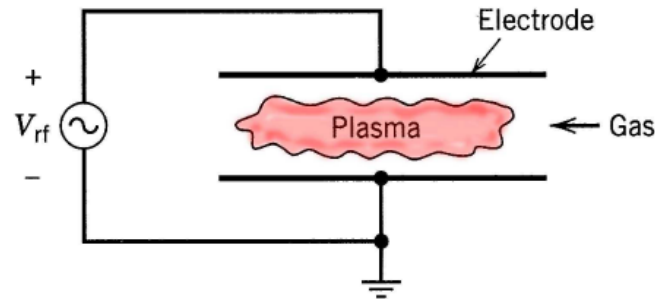
Charged particle collisions with neutral particles are important

There are boundaries at which surface losses are important

The electrons are not in thermal equilibrium with the ions



(a)



(b)

- Device sizes $\sim 30 \text{ cm} - 1 \text{ m}$
- Frequencies from DC to rf (13.56 MHz) to microwaves (2.45 GHz)

UNITS AND CONSTANTS

- SI units: meters (m), kilograms (kg), seconds (s), coulombs (C)
 $e = 1.6 \times 10^{-19}$ C, electron charge = $-e$

- Energy unit is joule (J)

Often use electron-volt

$$1 \text{ eV} = 1.6 \times 10^{-19} \text{ J}$$

- Temperature unit is kelvin (K)

Often use equivalent voltage of the temperature

$$T_e(\text{volts}) = \frac{kT_e(\text{kelvins})}{e}$$

where k = Boltzmann's constant = 1.38×10^{-23} J/K

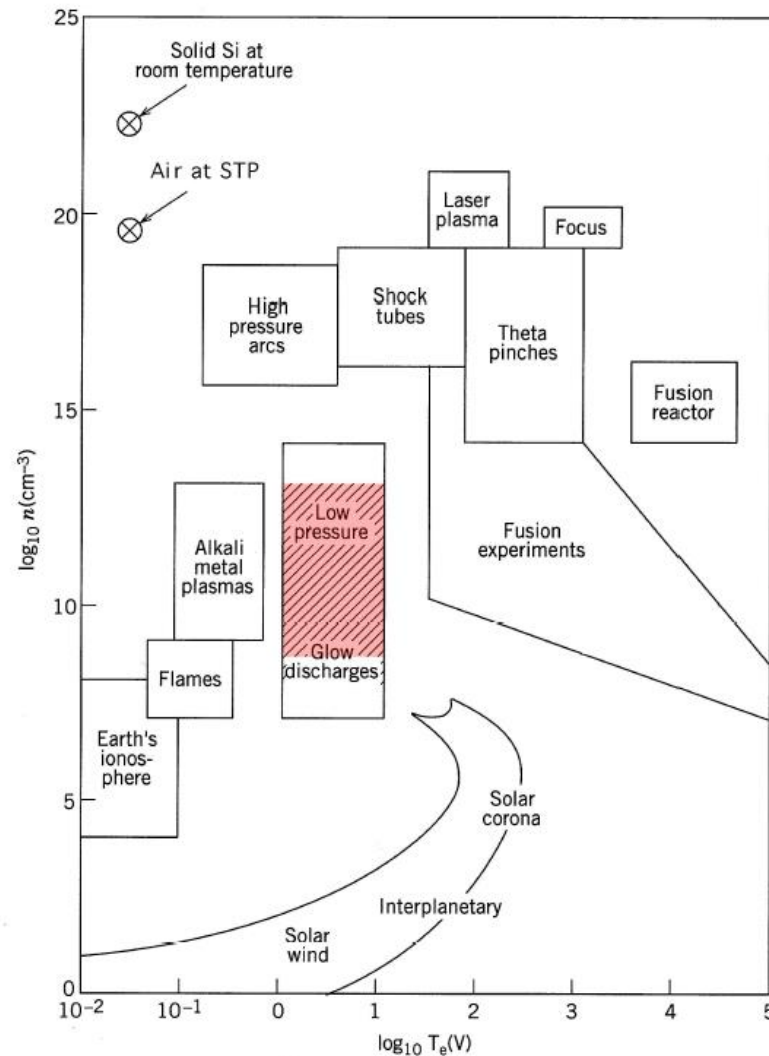
$$1 \text{ V} \Longleftrightarrow 11,600 \text{ K}$$

- Pressure unit is pascal (Pa); $1 \text{ Pa} = 1 \text{ N/m}^2$

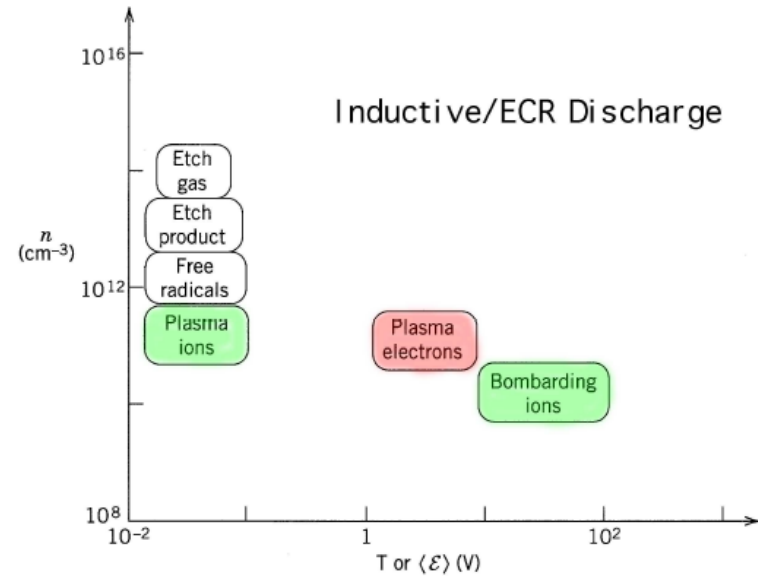
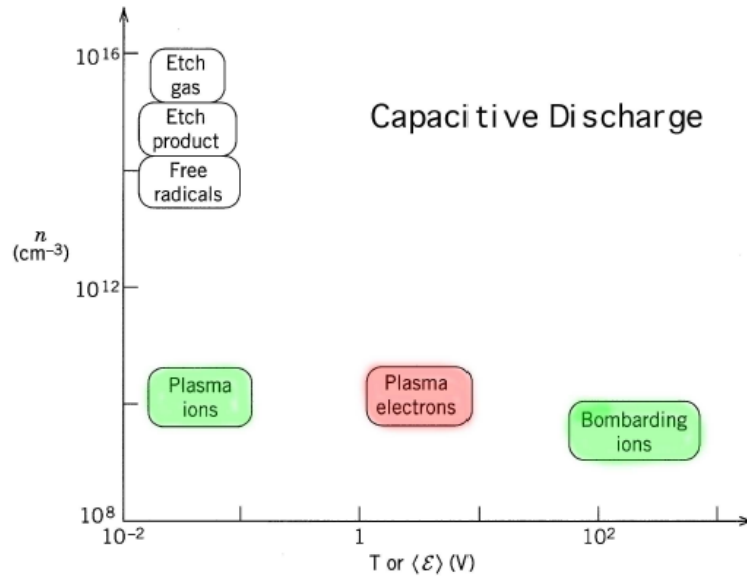
Atmospheric pressure $\equiv 1 \text{ bar} \approx 10^5 \text{ Pa} \approx 760 \text{ Torr}$

$$1 \text{ Pa} \Longleftrightarrow 7.5 \text{ mTorr}$$

PLASMA DENSITY VERSUS TEMPERATURE

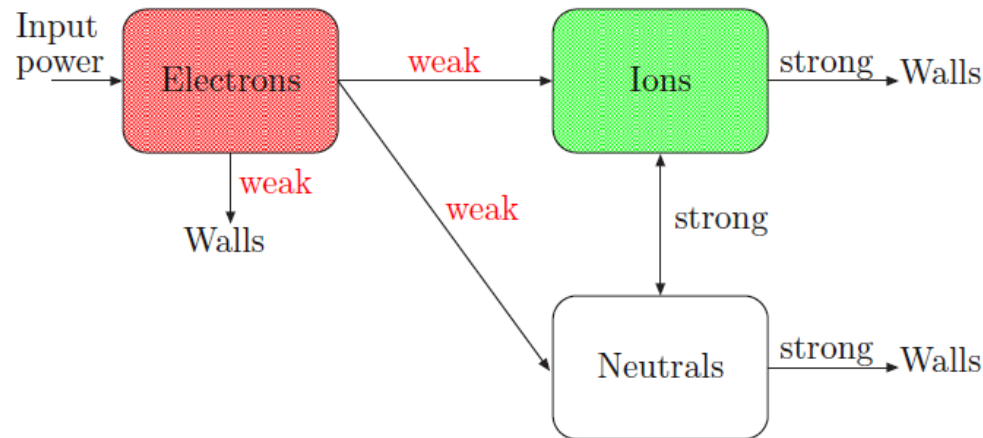


RELATIVE DENSITIES AND ENERGIES



NON-EQUILIBRIUM

- Energy coupling between electrons and heavy particles is weak



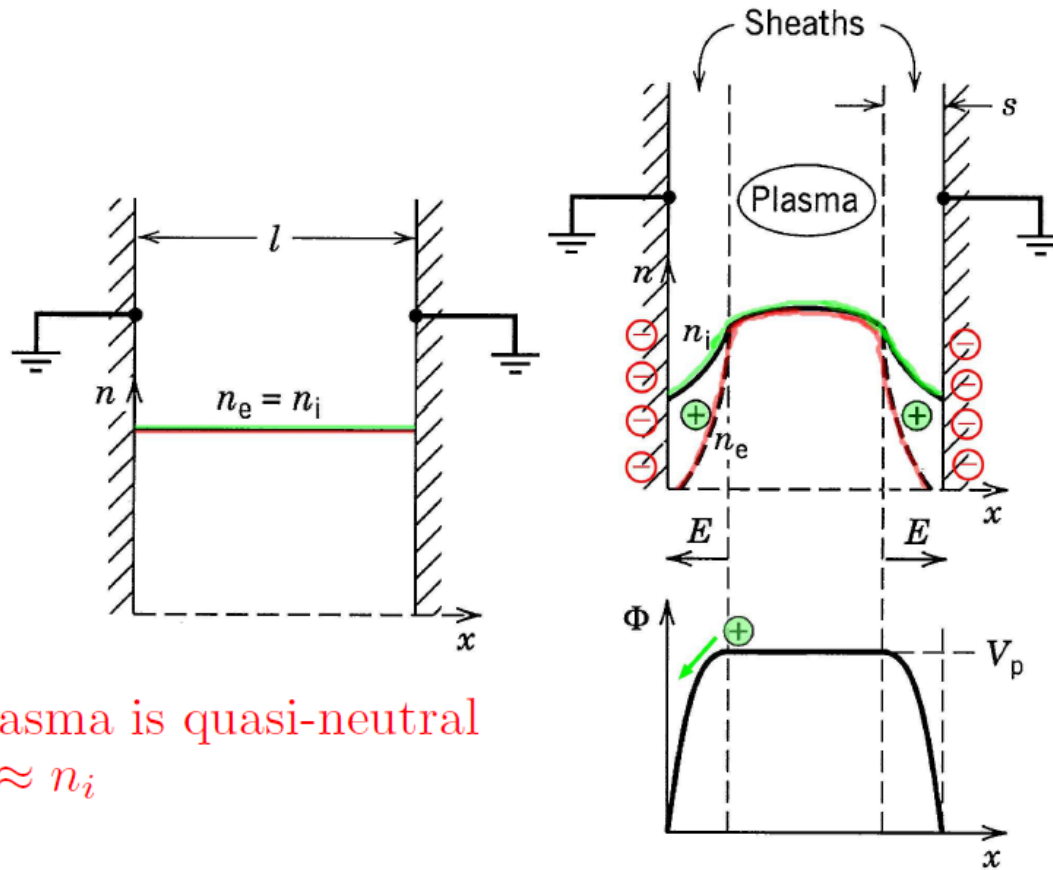
- Electrons are *not* in thermal equilibrium with ions or neutrals

$$T_e \gg T_i \quad \text{in plasma bulk}$$
$$\text{Bombarding ion } \mathcal{E}_i \gg T_e \quad \text{at wafer surface}$$

- “High temperature processing at low temperatures”
 - Wafer can be near room temperature
 - Electrons produce free radicals \Rightarrow chemistry
 - Electrons produce electron-ion pairs \Rightarrow ion bombardment

ELEMENTARY DISCHARGE BEHAVIOR

- Uniform density of electrons and ions n_e and n_i at time $t = 0$
- Low mass warm electrons quickly drain to the wall, forming sheaths



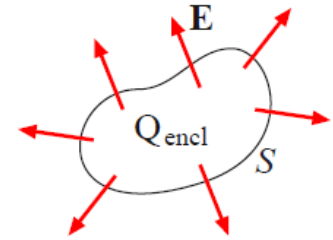
- Bulk plasma is quasi-neutral
 $\Rightarrow n_e \approx n_i$

- Ions accelerated to walls; ion bombarding energy $\mathcal{E}_i = \text{plasma-wall potential } V$

POISSON'S EQUATION

- An **electric field** can be generated by **charges**

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0} \quad \text{or} \quad \oiint_S \bar{\mathbf{E}} \cdot d\mathbf{A} = \frac{Q_{\text{encl}}}{\epsilon_0}$$



- For slow time variations (dc, rf, but not microwaves)

$$\mathbf{E} \approx -\nabla\Phi$$

\mathbf{E} = electric field (V/m), ρ = charge density (C/m³),

Φ = potential (V), $\epsilon_0 = 8.85 \times 10^{-12}$ F/m

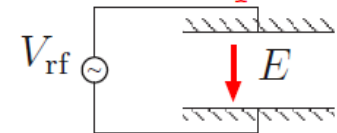
- In 1D planar geometry

$$\boxed{\frac{dE_x}{dx} = \frac{\rho}{\epsilon_0}, \quad \frac{d\Phi}{dx} = -E_x}$$

Combining these yields Poisson's equation

$$\boxed{\frac{d^2\Phi}{dx^2} = -\frac{\rho}{\epsilon_0}}$$

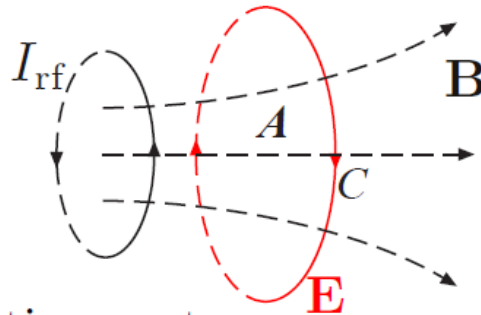
- This field powers a **capacitive discharge** or the **wafer bias power** of an inductive or ECR discharge



FARADAY'S LAW

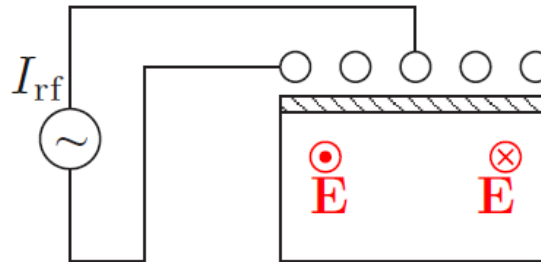
- An **electric field** can be generated by a **time-varying magnetic field**

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \quad \text{or} \quad \oint_C \mathbf{E} \cdot d\mathbf{l} = -\frac{\partial}{\partial t} \iint_A \mathbf{B} \cdot d\mathbf{A}$$



\mathbf{B} = magnetic induction vector

- This field powers the coil of an **inductive discharge** (top power)



AMPERE'S LAW

- Both **conduction currents** and **displacement currents** generate magnetic fields \mathbf{H}

$$\nabla \times \mathbf{H} = \mathbf{J}_c + \epsilon_0 \frac{\partial \mathbf{E}}{\partial t} = \mathbf{J} \quad [\text{A/m}^2]$$

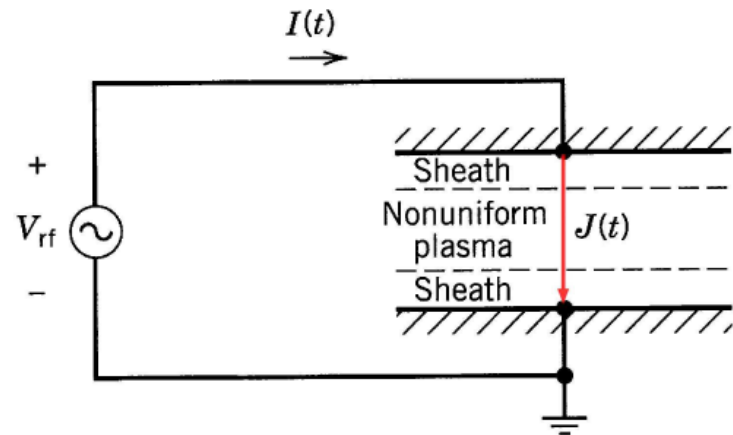
\mathbf{J}_c = conduction current density (physical motion of charges)

$\epsilon_0 \partial \mathbf{E} / \partial t$ = displacement current density (flows in vacuum)

\mathbf{J} = total current density

- Note the vector identity $\nabla \cdot (\nabla \times \mathbf{H}) = 0 \Rightarrow \nabla \cdot \mathbf{J} = 0$
- In 1D

$$\frac{\partial J(x, t)}{\partial x} = 0$$

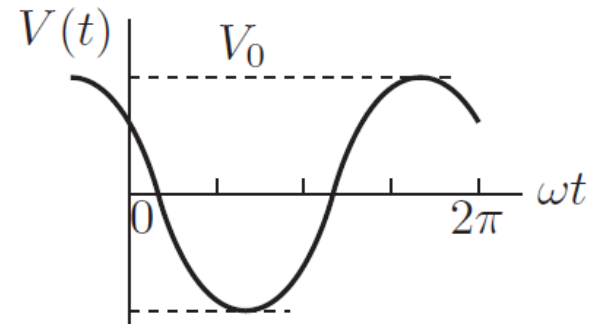


Total current J is independent of x

REVIEW OF PHASORS

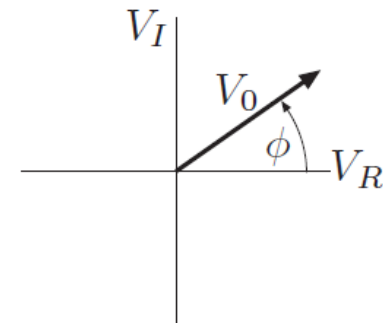
- **Physical voltage** (or current), a real sinusoidal function of time

$$V(t) = V_0 \cos(\omega t + \phi)$$



- **Phasor voltage** (or current), a complex number, independent of time

$$\tilde{V} = V_0 e^{j\phi} = V_R + jV_I$$



- Note that

$$V(t) = \text{Re} \left(\tilde{V} e^{j\omega t} \right)$$

- Hence

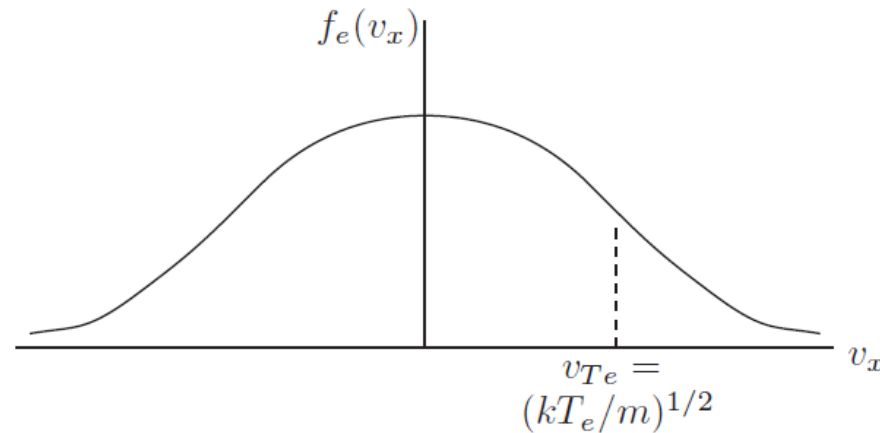
$$V(t) \Longleftrightarrow \tilde{V} \quad (\text{given } \omega)$$

THERMAL EQUILIBRIUM PROPERTIES

- **Electrons** generally near **thermal equilibrium**
Ions generally *not* in thermal equilibrium
- **Maxwellian** distribution of electrons

$$f_e(v) = n_e \left(\frac{m}{2\pi kT_e} \right)^{3/2} \exp \left(-\frac{mv^2}{2kT_e} \right)$$

where $v^2 = v_x^2 + v_y^2 + v_z^2$



- Pressure $p = nkT$
For neutral gas at room temperature (300 K)

$$n_g(\text{cm}^{-3}) \approx 3.3 \times 10^{16} p(\text{Torr})$$

AVERAGES OVER MAXWELLIAN DISTRIBUTION

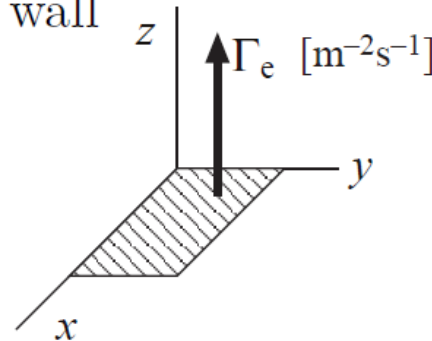
- Average energy

$$\left\langle \frac{1}{2} m v^2 \right\rangle = \frac{1}{n_e} \int d^3 v \frac{1}{2} m v^2 f_e(v) = \frac{3}{2} k T_e$$

- Average speed

$$\boxed{\bar{v}_e = \left(\frac{8 k T_e}{\pi m} \right)^{1/2}} \quad \left(= \frac{1}{n_e} \int d^3 v v f_e(v) \right)$$

- Average electron flux lost to a wall



$$\boxed{\Gamma_e = \frac{1}{4} n_e \bar{v}_e} \quad \left(= \int_{-\infty}^{\infty} dv_x \int_{-\infty}^{\infty} dv_y \int_0^{\infty} dv_z v_z f_e(v) \right)$$

- Average kinetic energy lost per electron lost to a wall

$$\boxed{\mathcal{E}_e = 2 T_e}$$

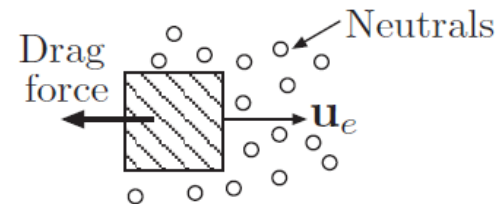
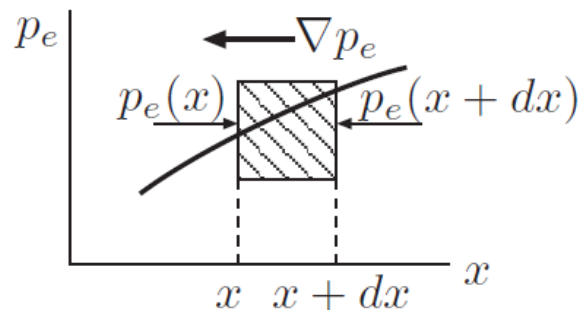
FORCES ON PARTICLES

- For a unit volume of electrons (or ions)

$$mn_e \frac{d\mathbf{u}_e}{dt} = qn_e \mathbf{E} - \nabla p_e - mn_e \nu_m \mathbf{u}_e$$

mass \times acceleration = electric field force +
+ pressure gradient force + friction (gas drag) force

- m = electron mass
 n_e = electron density
 \mathbf{u}_e = electron flow velocity
 $q = -e$ for electrons ($+e$ for ions)
 \mathbf{E} = electric field
 $p_e = n_e k T_e$ = electron pressure
 ν_m = collision frequency of electrons with neutrals [p. 36]



BOLTZMANN FACTOR FOR ELECTRONS

- If **electric field** and **pressure gradient** forces almost balance

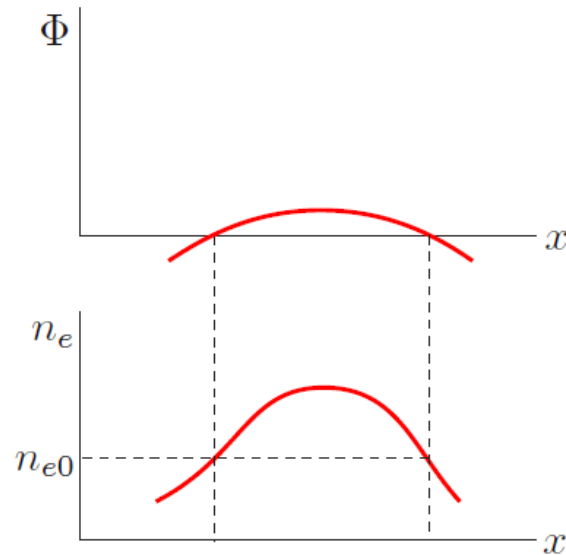
$$0 \approx -en_e \mathbf{E} - \nabla p_e$$

- Let $\mathbf{E} = -\nabla\Phi$ and $p_e = n_e kT_e$

$$\nabla\Phi = \frac{kT_e}{e} \frac{\nabla n_e}{n_e}$$

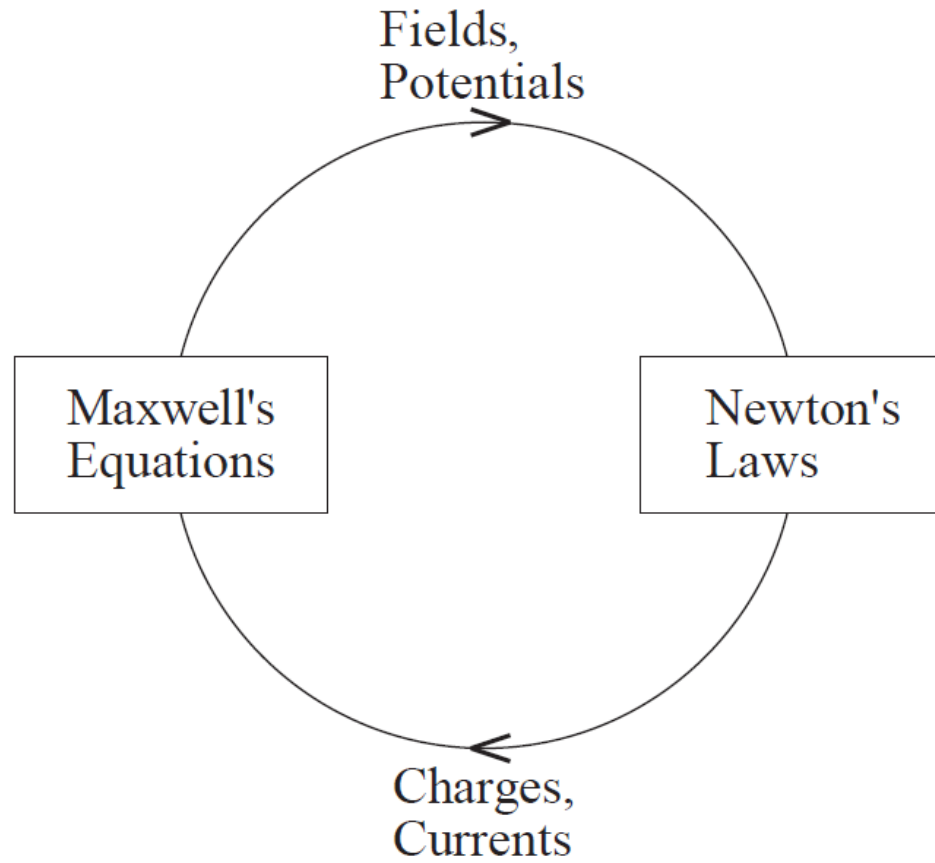
- Put $kT_e/e = T_e$ (volts) and integrate to obtain

$$n_e(\mathbf{r}) = n_{e0} e^{\Phi(\mathbf{r})/T_e}$$



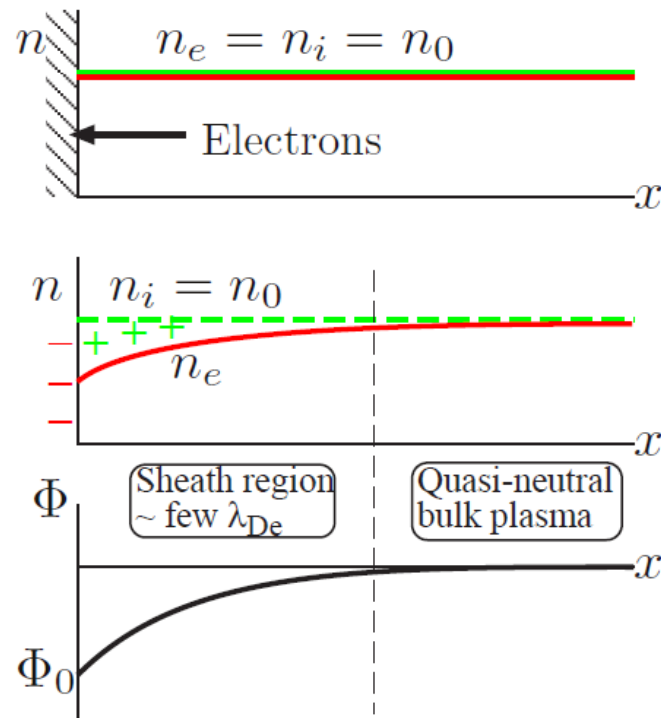
UNDERSTANDING PLASMA BEHAVIOR

- The field equations and the force equations are **coupled**



DEBYE LENGTH λ_{De}

- The **characteristic length scale** of a plasma
- Low voltage sheaths \sim few Debye lengths thick
- Let's consider how a sheath forms near a wall
Electrons leave plasma before ions and charge wall negative



Assume electrons in thermal equilibrium and stationary ions

DEBYE LENGTH λ_{De} (CONT'D)

- Newton's laws [p. 18]

$$n_e(x) = n_0 e^{\Phi/T_e}, \quad n_i = n_0$$

- Use in Poisson's equation [p. 12]

$$\frac{d^2\Phi}{dx^2} = -\frac{en_0}{\epsilon_0} \left(1 - e^{\Phi/T_e}\right)$$

- Linearize $e^{\Phi/T_e} \approx 1 + \Phi/T_e$

$$\frac{d^2\Phi}{dx^2} = \frac{en_0}{\epsilon_0 T_e} \Phi$$

- Solution is

$$\Phi(x) = \Phi_0 e^{-x/\lambda_{De}},$$

$$\lambda_{De} = \left(\frac{\epsilon_0 T_e}{en_0} \right)^{1/2}$$

- In practical units

$$\lambda_{De}(\text{cm}) = 740 \sqrt{T_e/n_0}, \quad T_e \text{ in volts, } n_0 \text{ in cm}^{-3}$$

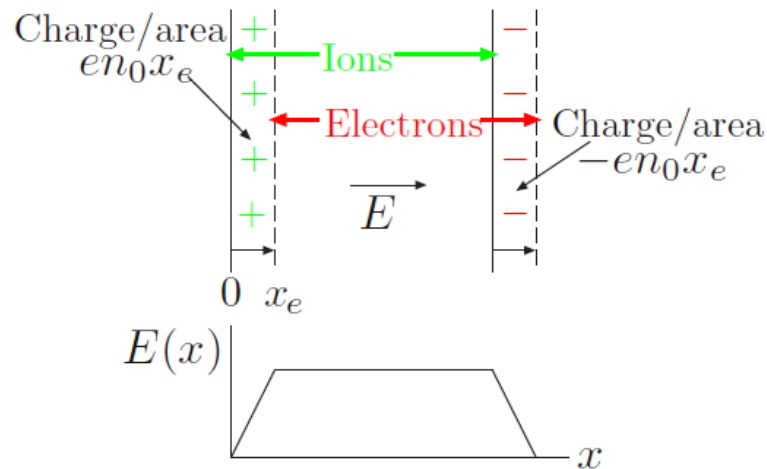
- Example

At $T_e = 1 \text{ V}$ and $n_0 = 10^{10} \text{ cm}^{-3}$, $\lambda_{De} = 7.4 \times 10^{-3} \text{ cm}$

\Rightarrow Sheath is $\sim 0.15 \text{ mm}$ thick (Very thin!)

ELECTRON PLASMA FREQUENCY ω_{pe}

- The **fundamental timescale** for a plasma
- Consider a plasma slab (no walls). Displace all electrons to the right a small distance x_{e0} , and release them



- Maxwell's equations (parallel plate capacitor) [p. 12]

$$E = \frac{en_0x_e(t)}{\epsilon_0}$$

ELECTRON PLASMA FREQUENCY ω_{pe} (CONT'D)

- Newton's laws (electron motion) [p. 18]

$$m \frac{d^2 x_e(t)}{dt^2} = -eE = -\frac{e^2 n_0}{\epsilon_0} x_e(t)$$

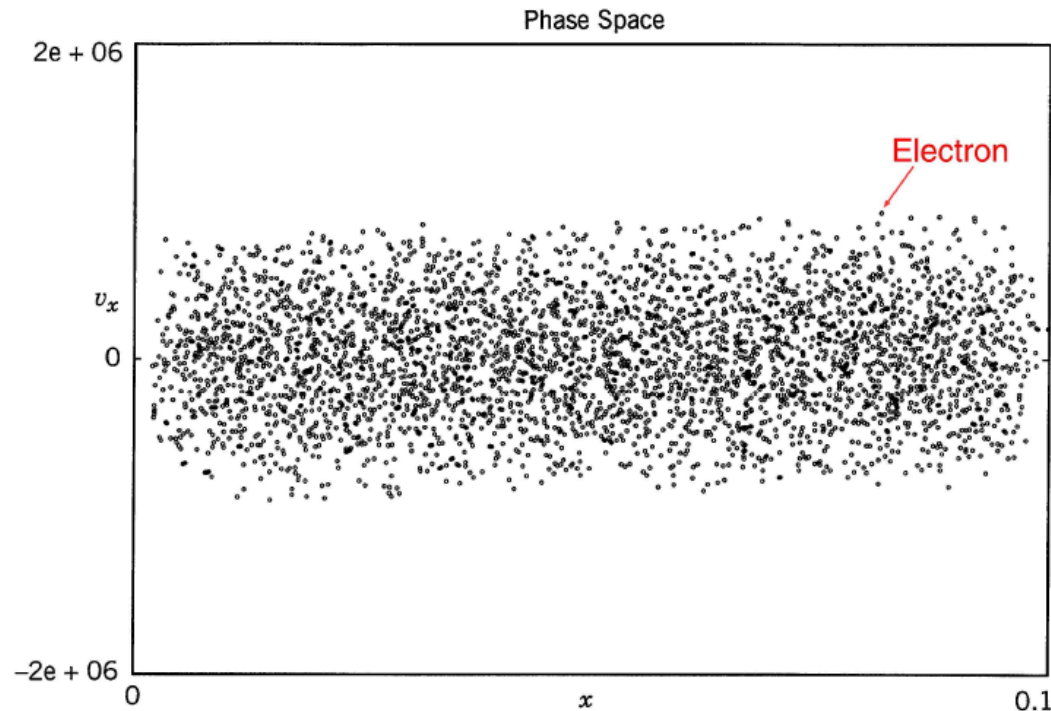
- Solution is electron plasma oscillations

$$x_e(t) = x_{e0} \cos \omega_{pe} t, \quad \boxed{\omega_{pe} = \left(\frac{e^2 n_0}{\epsilon_0 m} \right)^{1/2}}$$

- Practical formula is $f_{pe}(\text{Hz}) = 9000 \sqrt{n_0}$, n_0 in cm^{-3}
 \implies microwave frequencies ($\gtrsim 1 \text{ GHz}$) for typical plasmas

1D SIMULATION OF SHEATH FORMATION

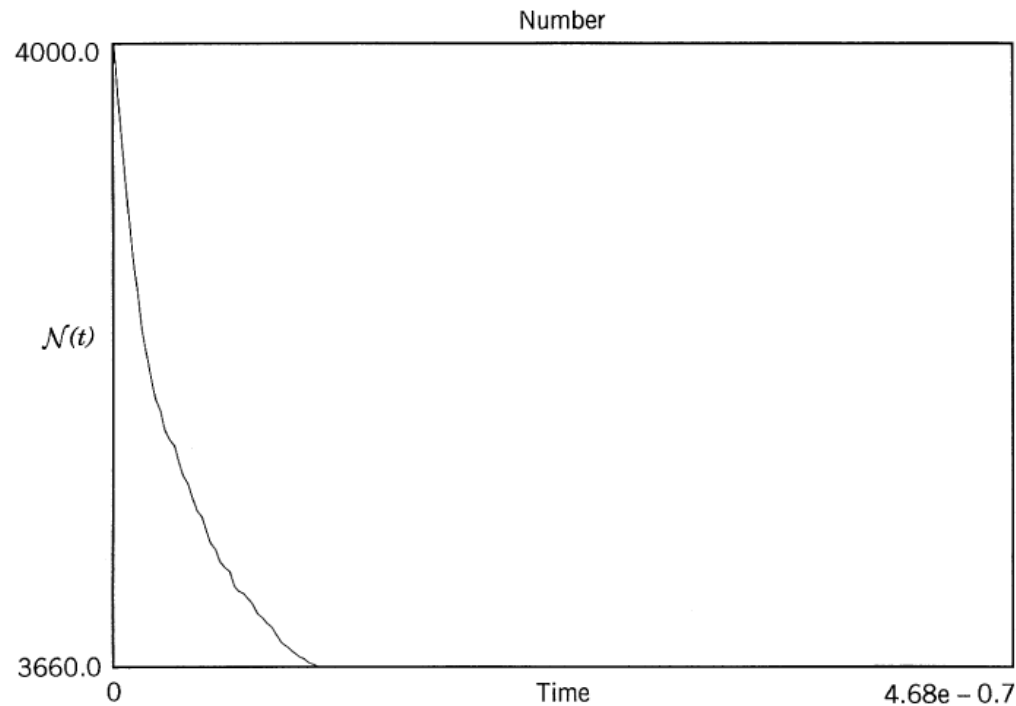
- Particle-in-cell (PIC) simulations with uniform fixed ion density; 4000 electron sheets; solve Newton's laws + Maxwell's equations
- $T_e = 1$ V (random), $n_e = n_i = 10^{13} \text{ m}^{-3}$ (low), $l = 0.1$ m
- Electron v_x - x phase space at $t = 0.77 \mu\text{s}$



- Note absence of electron sheets near the walls

1D SIMULATION OF SHEATH FORMATION (CONT'D)

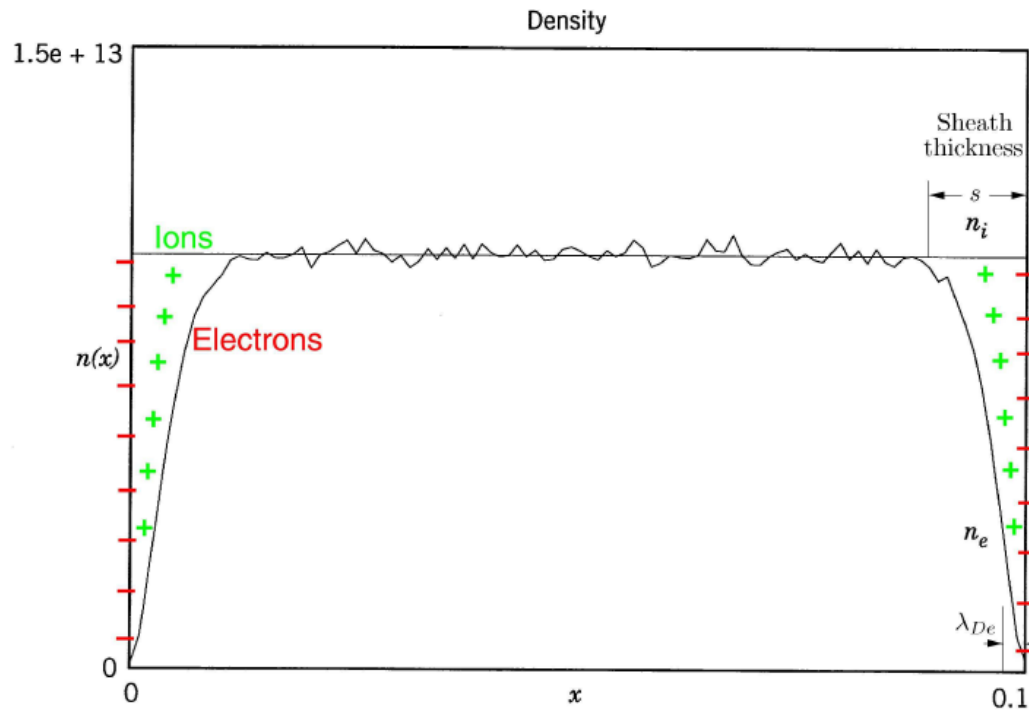
- Electron number \mathcal{N} versus t



- Note 340 electron sheets lost to walls to form sheaths

1D SIMULATION OF SHEATH FORMATION (CONT'D)

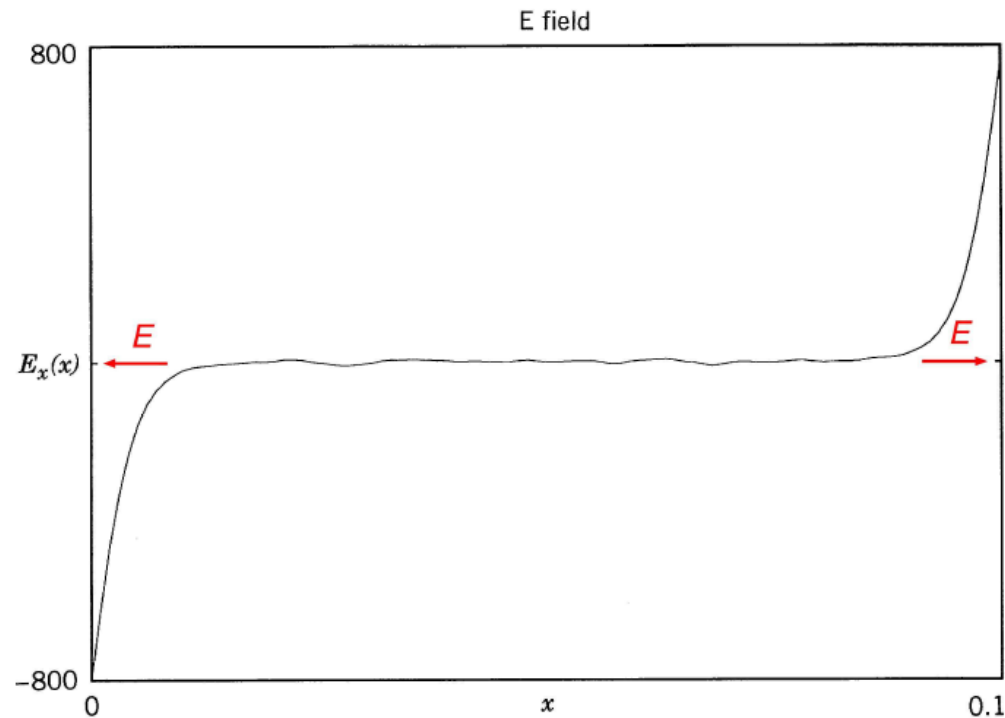
- Electron density $n_e(x)$ at $t = 0.77 \mu s$



- Note sheath width is a few Debye lengths

1D SIMULATION OF SHEATH FORMATION (CONT'D)

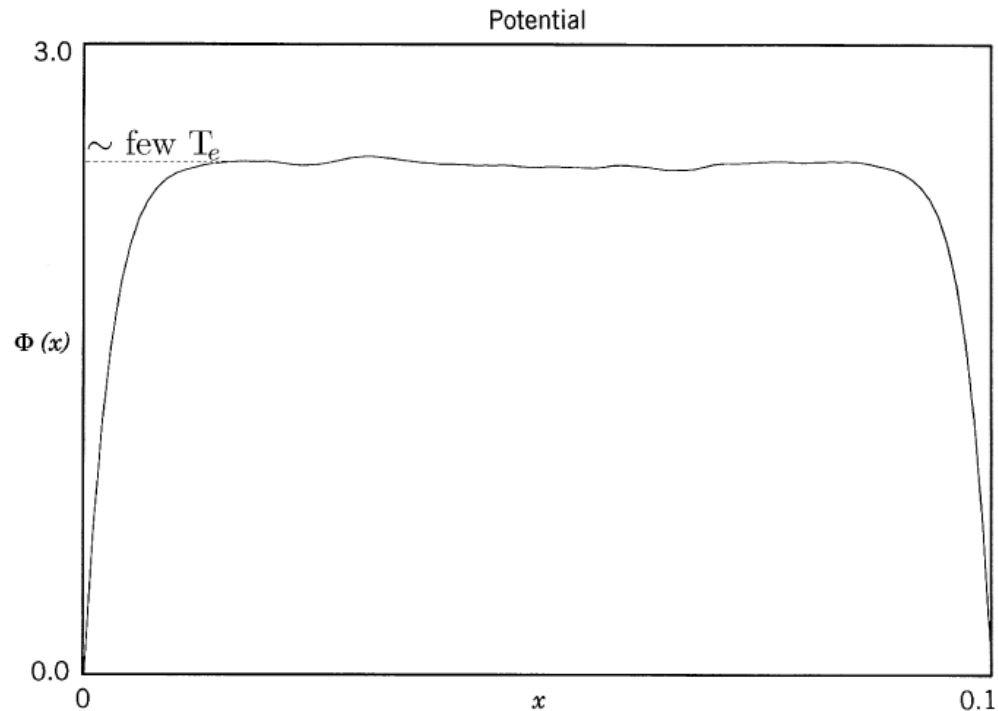
- Electric field $E(x)$ at $t = 0.77 \mu s$



- Note electric field retards electrons, accelerates ion into walls

1D SIMULATION OF SHEATH FORMATION (CONT'D)

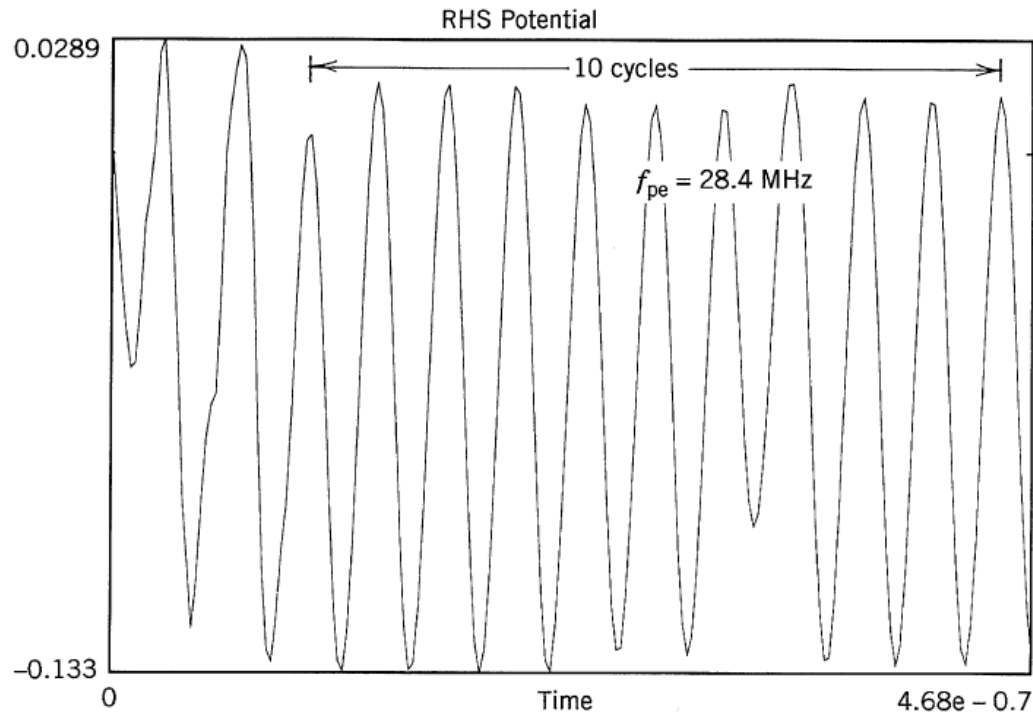
- Potential $\Phi(x)$ at $t = 0.77 \mu s$



- Note plasma potential builds up to a few T_e with respect to wall

1D SIMULATION OF SHEATH FORMATION (CONT'D)

- Right hand potential $\Phi(x = l)$ versus t



- Due to asymmetric electron initial conditions, a small oscillation of the right hand potential is excited at the plasma frequency

PLASMA DIELECTRIC CONSTANT ϵ_p

- RF discharges are driven at a frequency ω

$$E(t) = \text{Re}(\tilde{E} e^{j\omega t}), \quad \text{etc. [p. 15]}$$

- Define ϵ_p from the total current in Maxwell's equations [p. 14]

$$\nabla \times \tilde{H} = \underbrace{\tilde{J}_c + j\omega\epsilon_0\tilde{E}}_{\text{Total current } \tilde{J}} \equiv j\omega\epsilon_p\tilde{E}$$

- Conduction current $\tilde{J}_c = -en_e\tilde{u}_e$ is due to electrons
- Newton's law (electric field and neutral drag) is [p. 18]

$$j\omega m\tilde{u}_e = -e\tilde{E} - m\nu_m\tilde{u}_e$$

- Solve for \tilde{u}_e and evaluate \tilde{J}_c to obtain

$$\epsilon_p \equiv \epsilon_0\kappa_p = \epsilon_0 \left[1 - \frac{\omega_{pe}^2}{\omega(\omega - j\nu_m)} \right]$$

with $\omega_{pe} = (e^2 n_e / \epsilon_0 m)^{1/2}$ the electron plasma frequency [p. 23]

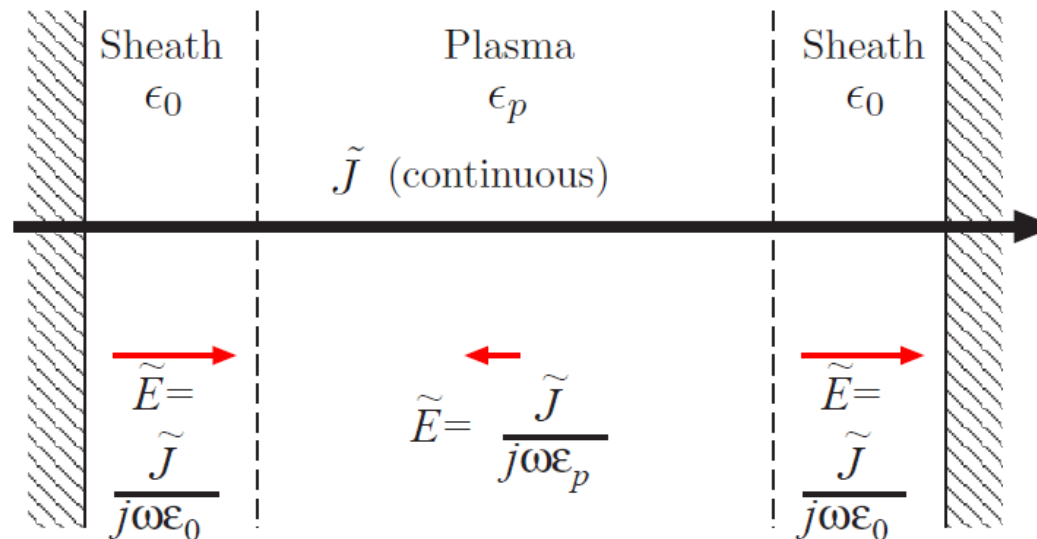
- For $\omega \gg \nu_m$, ϵ_p is mainly real (nearly lossless dielectric)
For $\nu_m \gg \omega$, ϵ_p is mainly imaginary (very lossy dielectric)

RF FIELDS IN LOW PRESSURE DISCHARGES

- Consider mainly lossless plasma ($\omega \gg \nu_m$)

$$\epsilon_p = \epsilon_0 \left(1 - \frac{\omega_{pe}^2}{\omega^2} \right)$$

- For rf discharges, $\omega_{pe} \gg \omega \implies \epsilon_p$ is negative ($\epsilon_p = -1000 \epsilon_0$)
- RF current density \tilde{J} is continuous across the discharge [p. 14]



- Electric field in plasma is $1000 \times$ smaller than in sheaths!
- Although field in plasma is small, it sustains the plasma!

PLASMA CONDUCTIVITY σ_p

- It is useful to introduce rf plasma conductivity $\tilde{J}_c \equiv \sigma_p \tilde{E}$
- Find \tilde{J}_c to be a linear function of \tilde{E} [p. 31]

$$\sigma_p = \frac{e^2 n_e}{m(\nu_m + j\omega)}$$

- DC plasma conductivity ($\omega \ll \nu_m$)

$$\sigma_{dc} = \frac{e^2 n_e}{m\nu_m}$$

- The plasma dielectric constant and conductivity are related by
$$j\omega\epsilon_p = \sigma_p + j\omega\epsilon_0$$
- RF current flowing through the plasma heats electrons (just like a resistor)

OHMIC HEATING POWER

- Time average power absorbed/volume

$$p_d = \langle \mathbf{J}(t) \cdot \mathbf{E}(t) \rangle = \frac{1}{2} \operatorname{Re} (\tilde{J} \cdot \tilde{E}^*) \quad [\text{W/m}^3]$$

Here $\tilde{E}^* =$ complex conjugate of \tilde{E}

- Since \tilde{J} is the same everywhere in the discharge [p. 32], put $\tilde{E} = \tilde{J}/j\omega\epsilon_p$ to find p_d in terms of \tilde{J} alone
- For discharges with $\omega \ll \omega_{pe}$ (all rf discharges)

$$p_d = \frac{1}{2} |\tilde{J}|^2 \frac{1}{\sigma_{dc}} \quad [\text{W/m}^3]$$

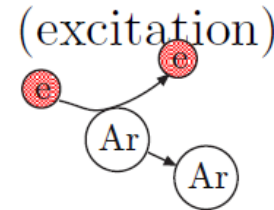
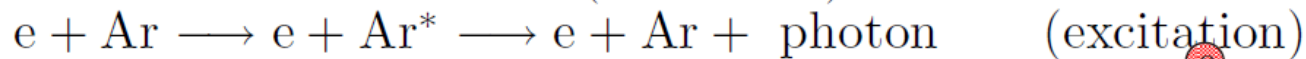
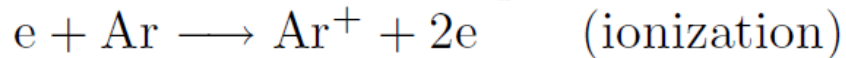
ELECTRON COLLISIONS WITH ARGON

- Maxwellian electrons collide with Ar atoms (density n_g)

$$\frac{\# \text{ collisions of a particular kind}}{\text{s-m}^3} = \nu n_e = K n_g n_e$$

ν = collision frequency [s^{-1}], $K(T_e)$ = rate coefficient [m^3/s]

- Electron-Ar collision processes

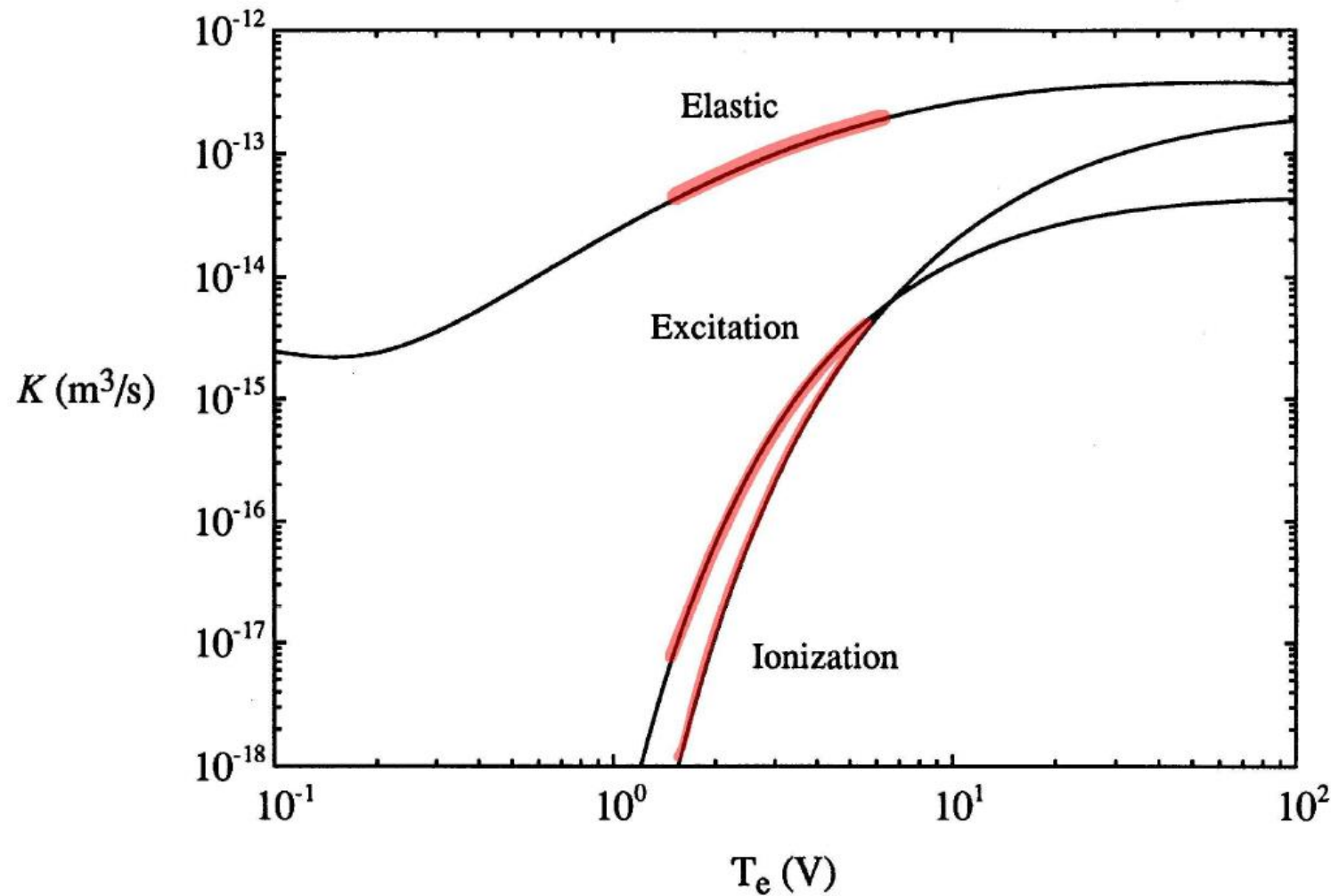


- Rate coefficient $K(T_e)$ is average of cross section $\sigma(v_R)$ [m^2] for process, over Maxwellian distribution

$$K(T_e) = \langle \sigma v_R \rangle_{\text{Maxwellian}}$$

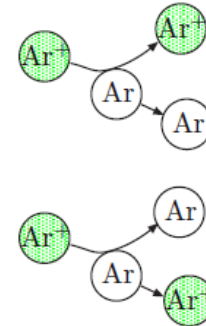
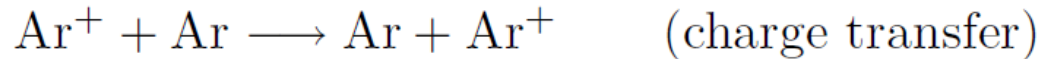
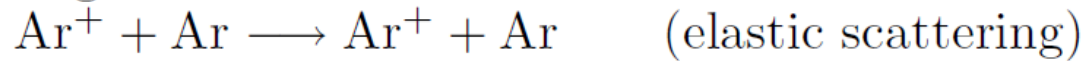
v_R = relative velocity of colliding particles

ELECTRON-ARGON RATE COEFFICIENTS



ION COLLISIONS WITH ARGON

- Argon ions collide with Ar atoms



- Total cross section for room temperature ions $\sigma_i \approx 10^{-14} \text{ cm}^2$
- Ion-neutral mean free path (distance ion travels before colliding)

$$\lambda_i = \frac{1}{n_g \sigma_i}$$

- Practical formula

$$\lambda_i(\text{cm}) = \frac{1}{330 p}, \quad p \text{ in Torr}$$

- Ion-neutral collision frequency

$$\nu_i = \frac{\bar{v}_i}{\lambda_i}$$

$$\text{with } \bar{v}_i = (8kT_i/\pi M)^{1/2}$$

THREE ENERGY LOSS PROCESSES

1. Collisional energy \mathcal{E}_c lost per electron-ion pair created

$$K_{iz}\mathcal{E}_c = K_{iz}\mathcal{E}_{iz} + K_{ex}\mathcal{E}_{ex} + K_{el}(2m/M)(3T_e/2)$$

$$\implies \mathcal{E}_c(T_e) \quad (\text{voltage units})$$

\mathcal{E}_{iz} , \mathcal{E}_{ex} , and $(3m/M)T_e$ are energies lost by an electron due to an ionization, excitation, and elastic scattering collision

2. Electron kinetic energy lost to walls [p. 17]

$$\mathcal{E}_e = 2 T_e$$

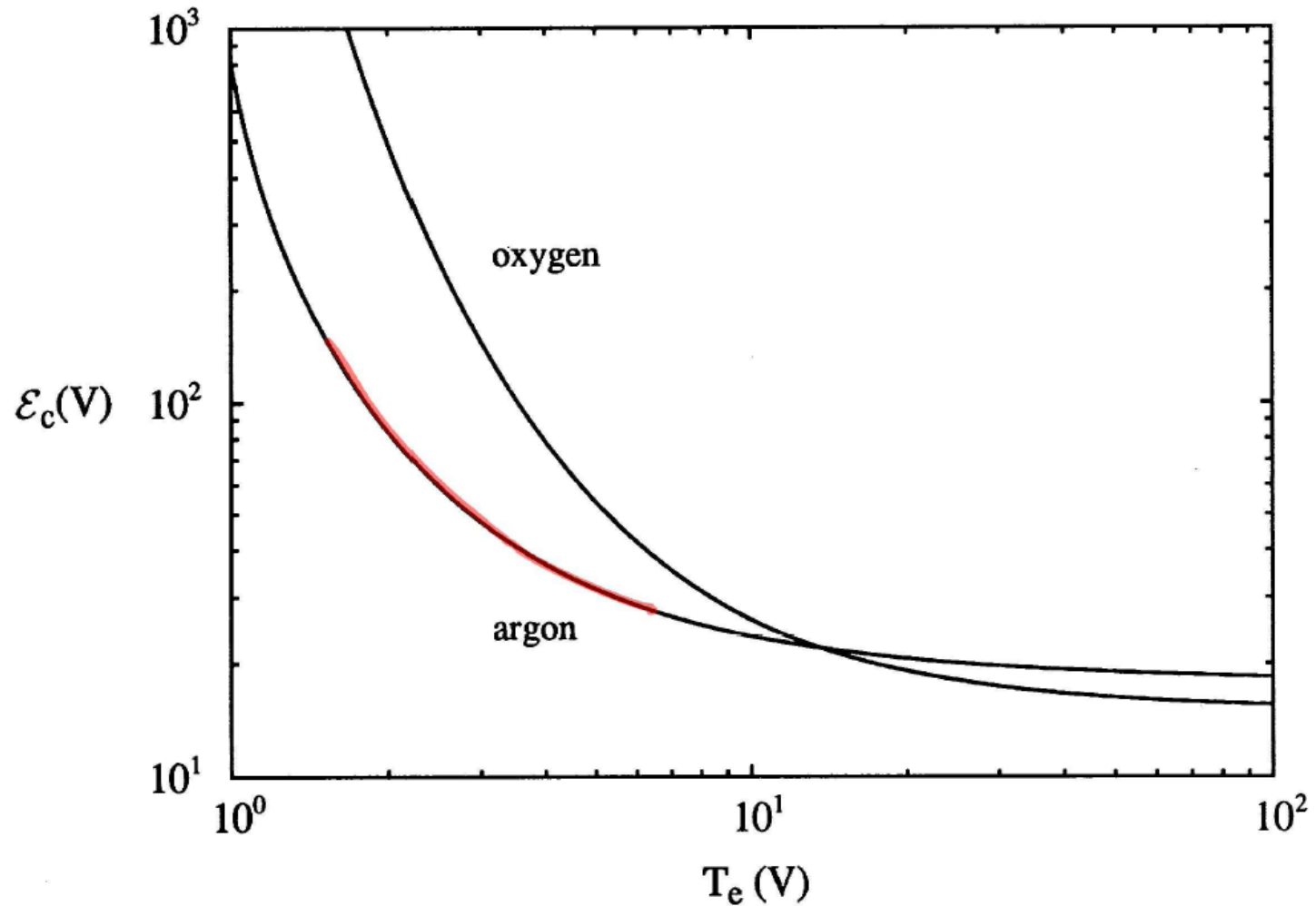
3. Ion kinetic energy lost to walls is mainly due to the dc potential \bar{V}_s across the sheath

$$\mathcal{E}_i \approx \bar{V}_s$$

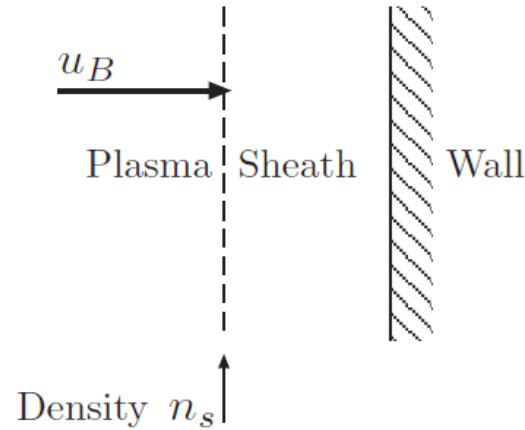
- Total energy lost per electron-ion pair lost to walls

$$\boxed{\mathcal{E}_T = \mathcal{E}_c + \mathcal{E}_e + \mathcal{E}_i}$$

COLLISIONAL ENERGY LOSSES



BOHM (ION LOSS) VELOCITY u_B



- Due to formation of a “presheath”, ions arrive at the plasma-sheath edge with directed energy $kT_e/2$

$$\frac{1}{2}Mu_B^2 = \frac{kT_e}{2}$$

- Electron-ion pairs are lost at the Bohm velocity at the plasma-sheath edge (density n_s)

$$\Gamma_{\text{wall}} = n_s u_B, \quad u_B = \left(\frac{kT_e}{M} \right)^{1/2}$$

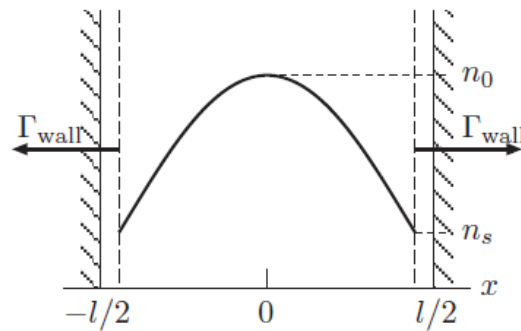
AMBIPOLAR DIFFUSION AT HIGH PRESSURES

- Plasma bulk is quasi-neutral ($n_e \approx n_i = n$) and the **electron and ion loss fluxes are equal** ($\Gamma_e \approx \Gamma_i \approx \Gamma$)
- Fick's law

$$\Gamma = -D_a \nabla n$$

with ambipolar diffusion coefficient $D_a = kT_e / M\nu_i$

- Density profile is sinusoidal



- Loss flux to the wall is

$$\Gamma_{\text{wall}} = n_s u_B \equiv h_l n_0 u_B$$

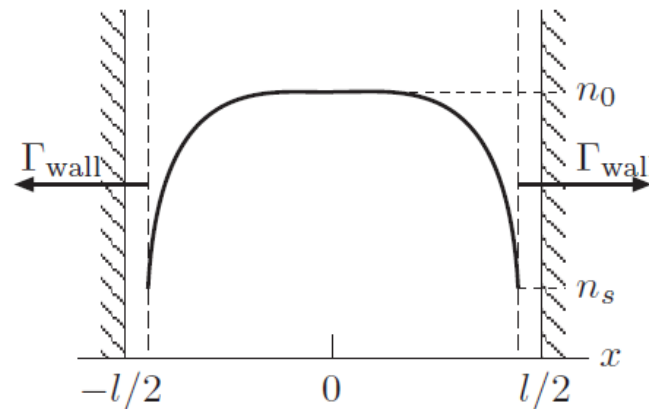
- From diffusion theory, edge-to-center density ratio is

$$h_l \equiv \frac{n_s}{n_0} = \frac{\pi}{l} \frac{u_B}{\nu_i}$$

- Applies for pressures > 100 mTorr in argon

AMBIPOLAR DIFFUSION AT LOW PRESSURES

- The diffusion coefficient is not constant
- Density profile is relatively flat in the center and falls sharply near the sheath edge



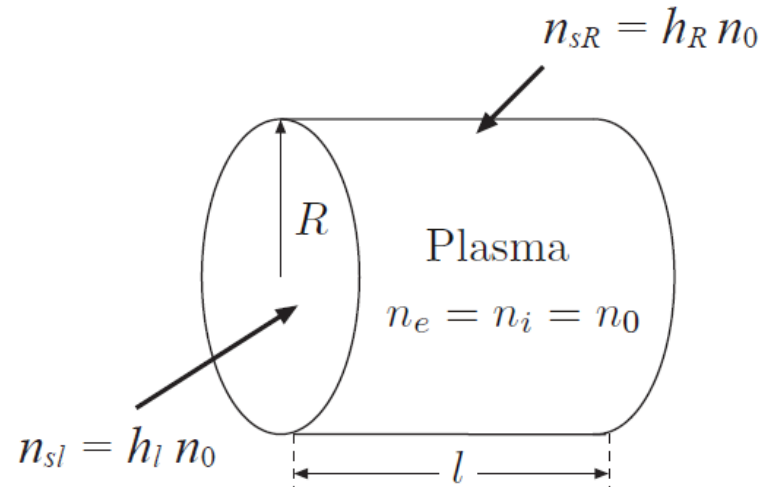
- The edge-to-center density ratio is

$$h_l \equiv \frac{n_s}{n_0} \approx \frac{0.86}{(3 + l/2\lambda_i)^{1/2}}$$

where λ_i = ion-neutral mean free path [p. 38]

- Applies for pressures < 100 mTorr in argon

AMBIPOLAR DIFFUSION IN LOW PRESSURE CYLINDRICAL DISCHARGE



- For a cylindrical plasma of length l and radius R , **loss fluxes to axial and radial walls** are

$$\Gamma_{\text{axial}} = h_l n_0 u_B, \quad \Gamma_{\text{radial}} = h_R n_0 u_B$$

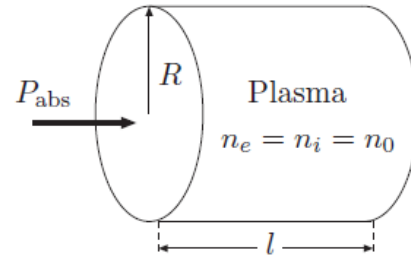
where the **edge-to-center density ratios** are

$$h_l \approx \frac{0.86}{(3 + l/2\lambda_i)^{1/2}}, \quad h_R \approx \frac{0.8}{(4 + R/\lambda_i)^{1/2}}$$

- Applies for pressures < 100 mTorr in argon

PARTICLE BALANCE AND T_e

- Assume uniform cylindrical plasma absorbing power P_{abs}



- Particle balance

Production due to ionization = loss to the walls

$$K_{\text{iz}} n_g n_0 \pi R^2 l = (2\pi R^2 h_l n_0 + 2\pi R l h_R n_0) u_B$$

- Solve to obtain

$$\frac{K_{\text{iz}}(T_e)}{u_B(T_e)} = \frac{1}{n_g d_{\text{eff}}}$$

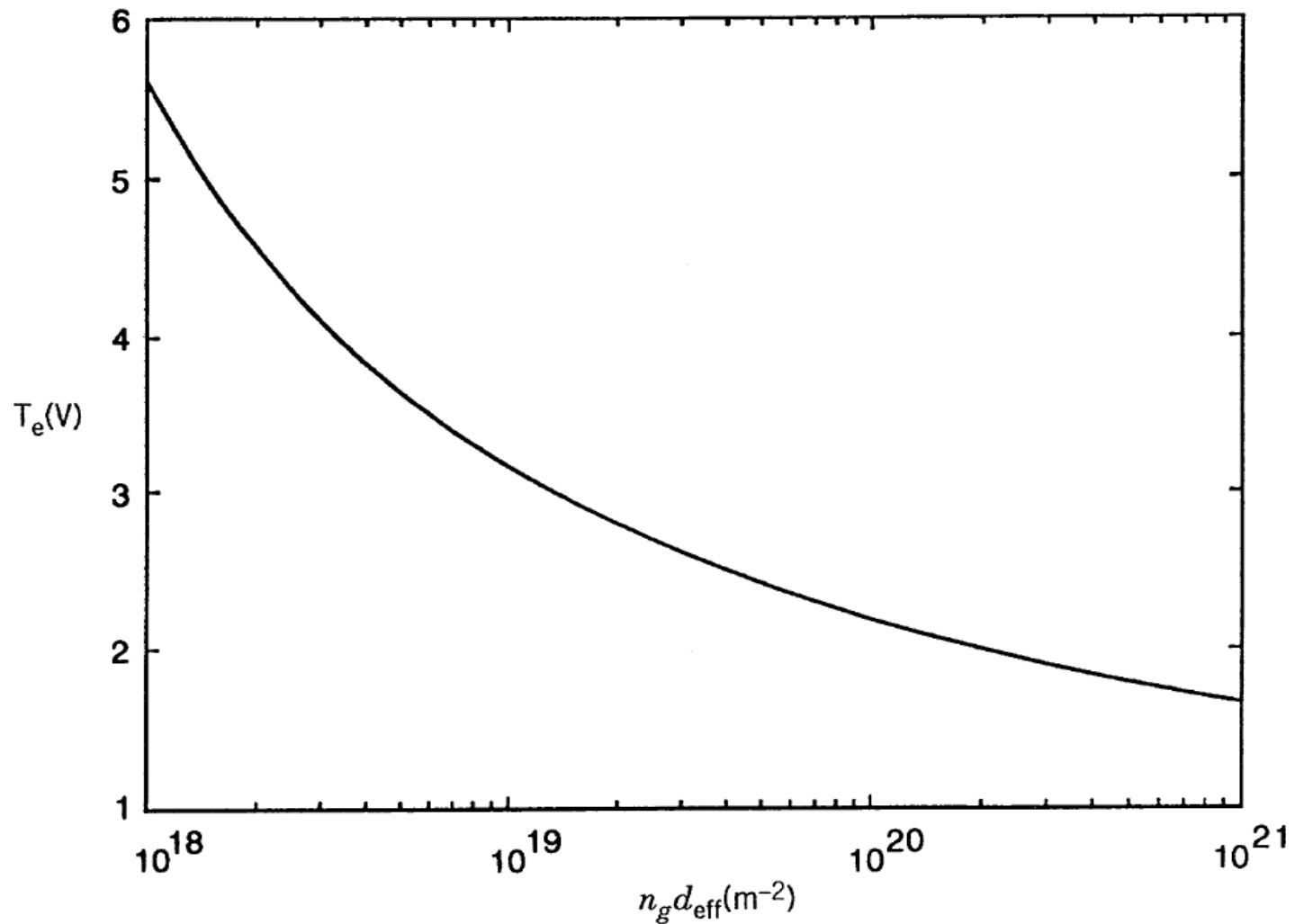
where

$$d_{\text{eff}} = \frac{1}{2} \frac{Rl}{Rh_l + lh_R}$$

is an effective plasma size

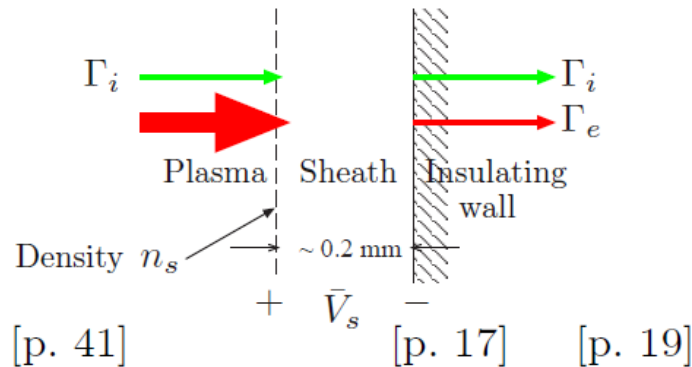
- Given n_g and $d_{\text{eff}} \Rightarrow$ electron temperature T_e
- T_e varies over a narrow range of 2–5 volts

ELECTRON TEMPERATURE IN ARGON DISCHARGE



ION ENERGY FOR LOW VOLTAGE SHEATHS

- \mathcal{E}_i = energy entering sheath + energy gained traversing sheath
- Ion energy entering sheath = $T_e/2$ (voltage units) [p. 41]
- Sheath voltage determined from particle conservation



$$\Gamma_i = n_s u_B, \quad \Gamma_e = \underbrace{\frac{1}{4} n_s \bar{v}_e}_{\text{Random flux at sheath edge}} e^{-\bar{V}_s/T_e}$$

with $\bar{v}_e = (8eT_e/\pi m)^{1/2}$

- The ion and electron fluxes at the wall must balance

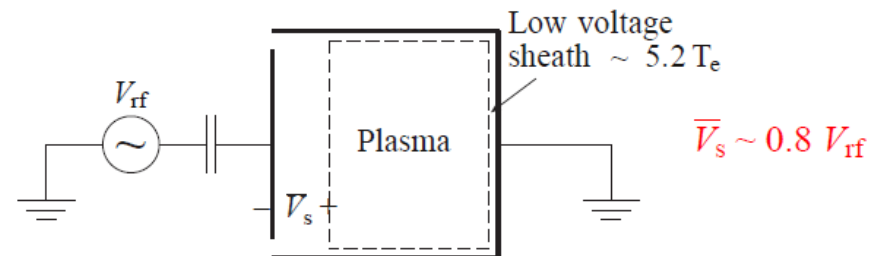
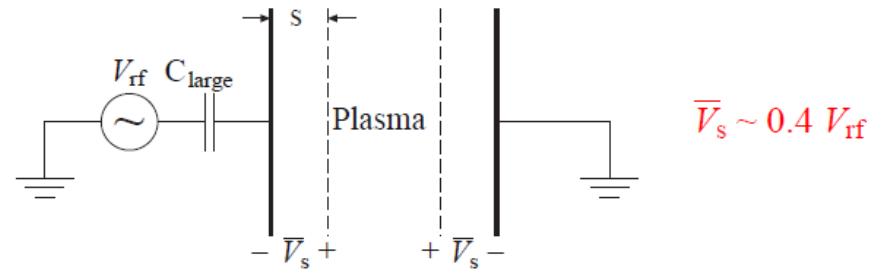
$$\bar{V}_s = \frac{T_e}{2} \ln \left(\frac{M}{2\pi m} \right)$$

or $\bar{V}_s \approx 4.7 T_e$ for argon

- Accounting for the initial ion energy, $\mathcal{E}_i \approx 5.2 T_e$

ION ENERGY FOR HIGH VOLTAGE SHEATHS

- Large ion bombarding energies can be gained near rf-driven electrodes embedded in the plasma



- The sheath thickness s (~ 0.5 cm) is given by the **Child Law**

$$\bar{J}_i = en_s u_B = \frac{4}{9} \epsilon_0 \left(\frac{2e}{M} \right)^{1/2} \frac{\bar{V}_s^{3/2}}{s^2}$$

- Estimating ion energy is not simple as it depends on the type of discharge and the application of bias voltages

POWER BALANCE AND n_0

- Assume low voltage sheaths at all surfaces

$$\mathcal{E}_T(T_e) = \underbrace{\mathcal{E}_c(T_e)}_{\text{Collisional}} + \underbrace{2 T_e}_{\text{Electron}} + \underbrace{5.2 T_e}_{\text{Ion}} \quad [\text{V}]$$

- Power balance

Power in = power out

$$P_{\text{abs}} = (h_l n_0 2\pi R^2 + h_R n_0 2\pi R l) u_B e \mathcal{E}_T \quad [\text{W}]$$

- Solve to obtain

$$n_0 = \frac{P_{\text{abs}}}{A_{\text{eff}} u_B e \mathcal{E}_T}$$

where

$$A_{\text{eff}} = 2\pi R^2 h_l + 2\pi R l h_R$$

is an effective area for particle loss

- Density n_0 is proportional to the absorbed power P_{abs}
- Density n_0 depends on pressure p through h_l , h_R , and T_e

PARTICLE AND POWER BALANCE

- Particle balance \implies electron temperature T_e
(independent of plasma density)
- Power balance \implies plasma density n_0
(once electron temperature T_e is known)

EXAMPLE 1

- Let $R = 0.15$ m, $l = 0.3$ m, $n_g = 3.3 \times 10^{19}$ m⁻³ ($p = 1$ mTorr at 300 K), and $P_{\text{abs}} = 800$ W
- Assume low voltage sheaths at all surfaces
- Find $\lambda_i = 0.03$ m [p. 38]. Then $h_l \approx h_R \approx 0.3$ [p. 44] and $d_{\text{eff}} \approx 0.17$ m [p. 46]
- T_e versus $n_g d_{\text{eff}}$ figure gives $T_e \approx 3.5$ V [p. 47]
- \mathcal{E}_c versus T_e figure gives $\mathcal{E}_c \approx 42$ V [p. 40]. Adding $\mathcal{E}_e = 2T_e \approx 7$ V and $\mathcal{E}_i \approx 5.2T_e \approx 18$ V yields $\mathcal{E}_T = 67$ V [p. 39]
- Find $u_B \approx 2.9 \times 10^3$ m/s [p. 41] and find $A_{\text{eff}} \approx 0.13$ m² [p. 50]
- Power balance yields $n_0 \approx 2.0 \times 10^{17}$ m⁻³ [p. 50]
- Ion current density $J_{il} = eh_l n_0 u_B \approx 2.9$ mA/cm² [p. 46]
- Ion bombarding energy $\mathcal{E}_i \approx 18$ V [p. 48]

EXAMPLE 2

- Apply a strong dc magnetic field along the cylinder axis
⇒ particle loss to radial wall is inhibited
- Assume no radial losses, then $d_{\text{eff}} = l/2h_l \approx 0.5 \text{ m}$
- From the T_e versus $n_g d_{\text{eff}}$ figure, $T_e \approx 3.3 \text{ V}$ (was 3.5 V)
- From the \mathcal{E}_c versus T_e figure, $\mathcal{E}_c \approx 46 \text{ V}$. Adding $\mathcal{E}_e = 2T_e \approx 6.6 \text{ V}$ and $\mathcal{E}_i \approx 5.2T_e \approx 17 \text{ V}$ yields $\mathcal{E}_T = 70 \text{ V}$
- Find $u_B \approx 2.8 \times 10^3 \text{ m/s}$ and find $A_{\text{eff}} = 2\pi R^2 h_l \approx 0.043 \text{ m}^2$
- Power balance yields $n_0 \approx 5.8 \times 10^{17} \text{ m}^{-3}$ (was $2 \times 10^{17} \text{ m}^{-3}$)
- Ion current density $J_{il} = eh_l n_0 u_B \approx 7.8 \text{ mA/cm}^2$
- Ion bombarding energy $\mathcal{E}_i \approx 17 \text{ V}$
⇒ Slight decrease in electron temperature T_e
⇒ Significant increase in plasma density n_0

EXPLAIN WHY!

- What happens to T_e and n_0 if there is a sheath voltage $V_s = 500 \text{ V}$ at each end plate?

CAPACITIVE RF DISCHARGES

SYMMETRIC HOMOGENEOUS MODEL

BASIC PROPERTIES

- Simplicity of concept
- RF rather than microwave powered
- Inherent high sheath voltages
- No independent control of plasma density and ion energy

- Control parameters

RF current \tilde{I}_{rf} (1–10 mA/cm²)

Driving frequency ω (2–13.56 MHz)

Neutral gas density n_g (10^{14} – 10^{16} cm⁻³)

Electrode separation l (1–10 cm)

- Discharge parameters to find

Plasma density n (10^9 – 10^{10} cm⁻³)

Electron temperature T_e (2–4 V)

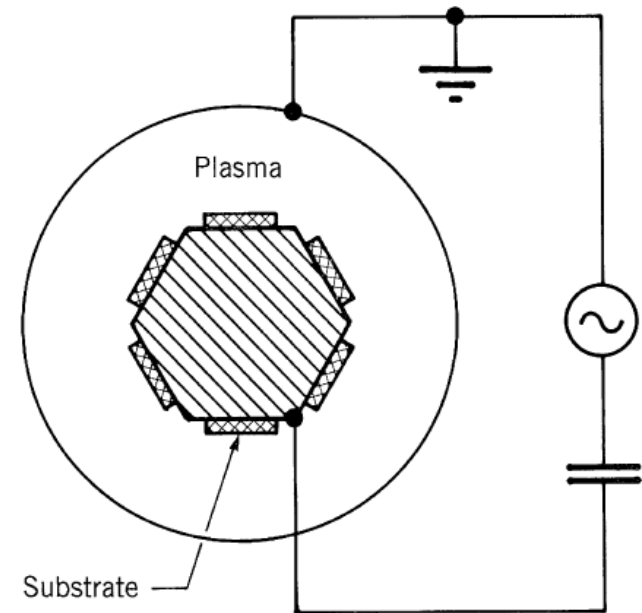
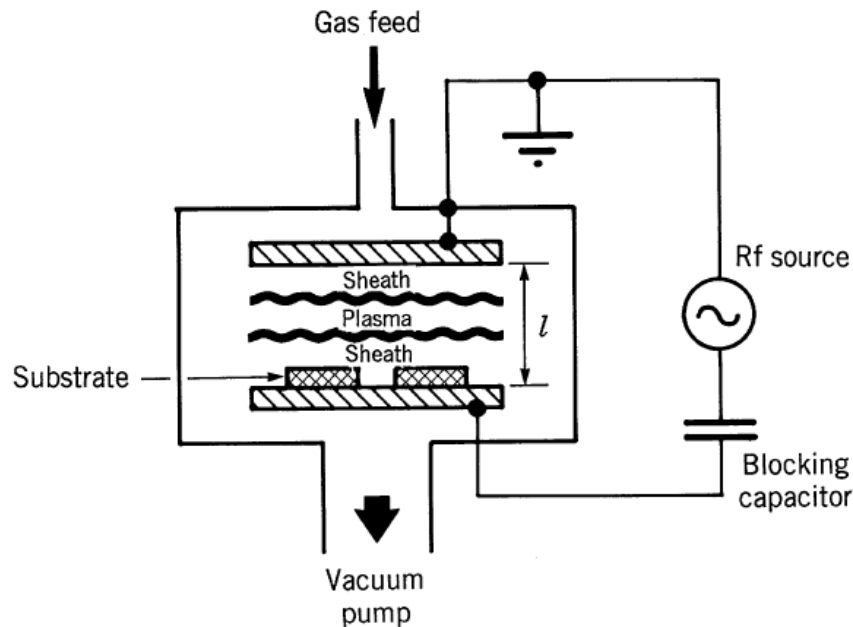
Discharge voltage V_{rf} (100–1000 V)

Discharge power P_{rf} (50–500 W)

Ion bombarding energy \mathcal{E}_i (50–500 V)

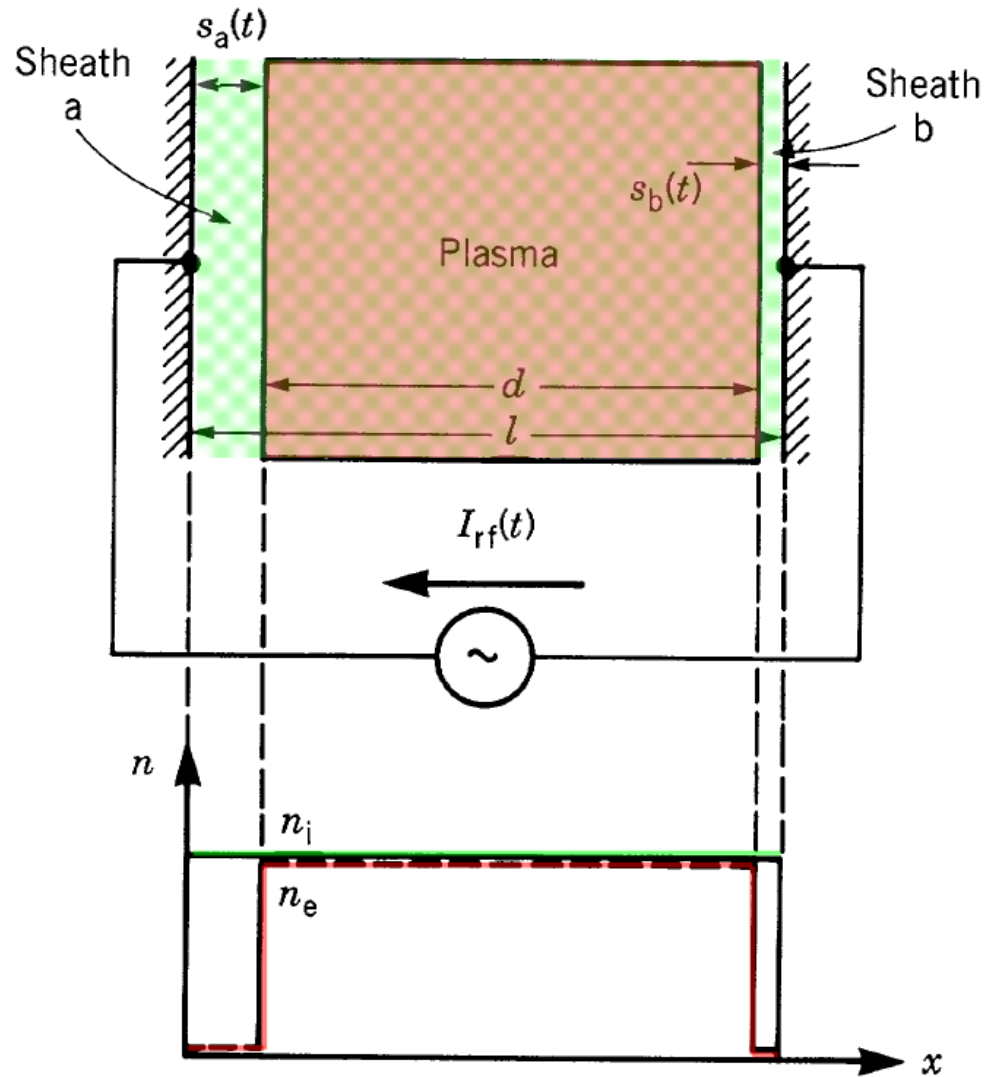
CONFIGURATIONS

- Multi-wafer parallel plate and “hex” configurations (1980’s)



- Modern configurations are single wafer parallel plate, sometimes driven at multiple rf frequencies

CURRENT-DRIVEN HOMOGENEOUS MODEL



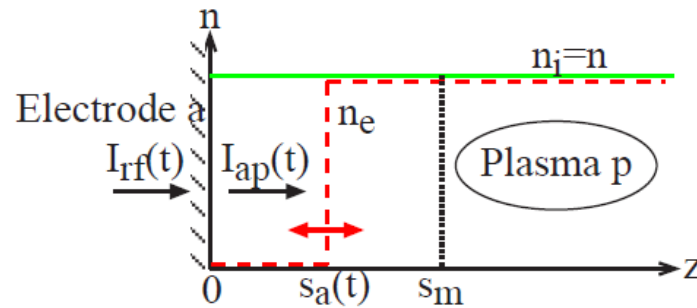
HOMOGENEOUS MODEL ASSUMPTIONS

- No transverse variations (along the electrodes)
- Electrons respond to instantaneous electric fields
- Ions respond to only time-average electric fields
- Electron density is zero in the sheath regions
- Ion density is constant in the plasma and sheath regions

$$n_i(z) = n_0$$

(We will correct this later)

ELECTRON SHEATH EDGE MOTION

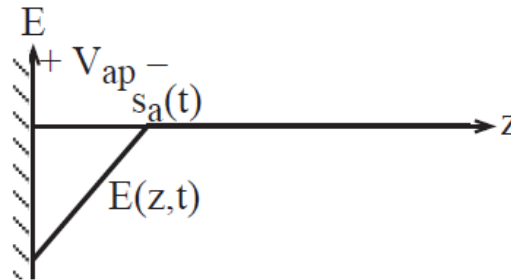


- The electric field is found by integrating the charge density in the sheath [p. 12]

$$\frac{dE}{dz} = \frac{en}{\epsilon_0}, \quad z < s_a(t)$$

to obtain

$$E(z, t) = \frac{en}{\epsilon_0} (z - s_a(t))$$



ELECTRON SHEATH EDGE MOTION (CONT'D)

- The displacement current in the sheath is [p. 14]

$$I_{ap} = \epsilon_0 A \frac{\partial E}{\partial t} = -enA \frac{ds_a}{dt}$$

- Let $I_{rf}(t) = \tilde{I}_0 \cos \omega t$ and integrate to obtain

$$s_a(t) = \bar{s}_0 - \tilde{s}_0 \sin \omega t$$

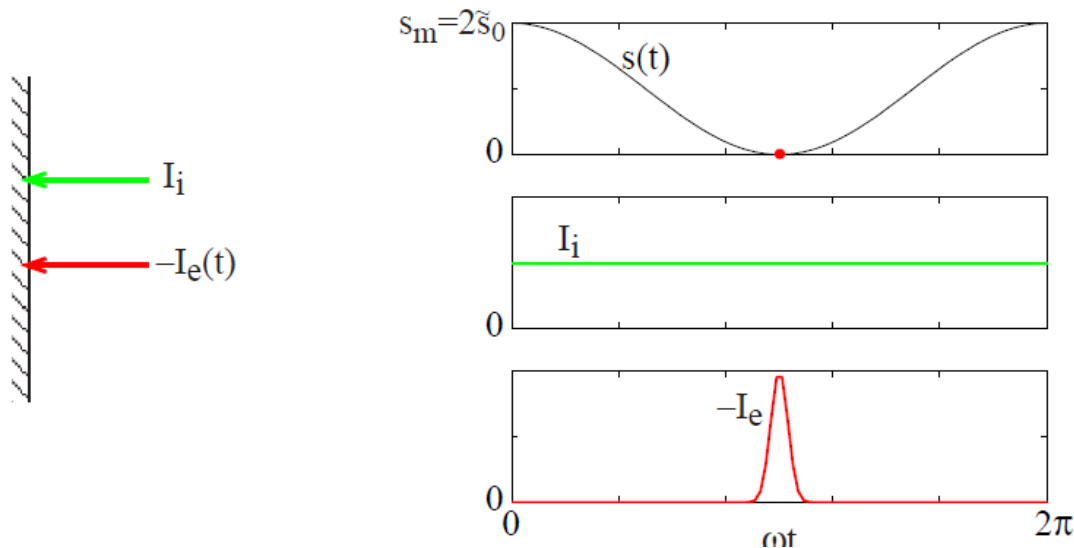
$$\tilde{s}_0 = \frac{\tilde{I}_0}{en\omega A}$$

- The oscillation amplitude of the sheath motion is \tilde{s}_0 , but what is the “constant of integration” \bar{s}_0 ?

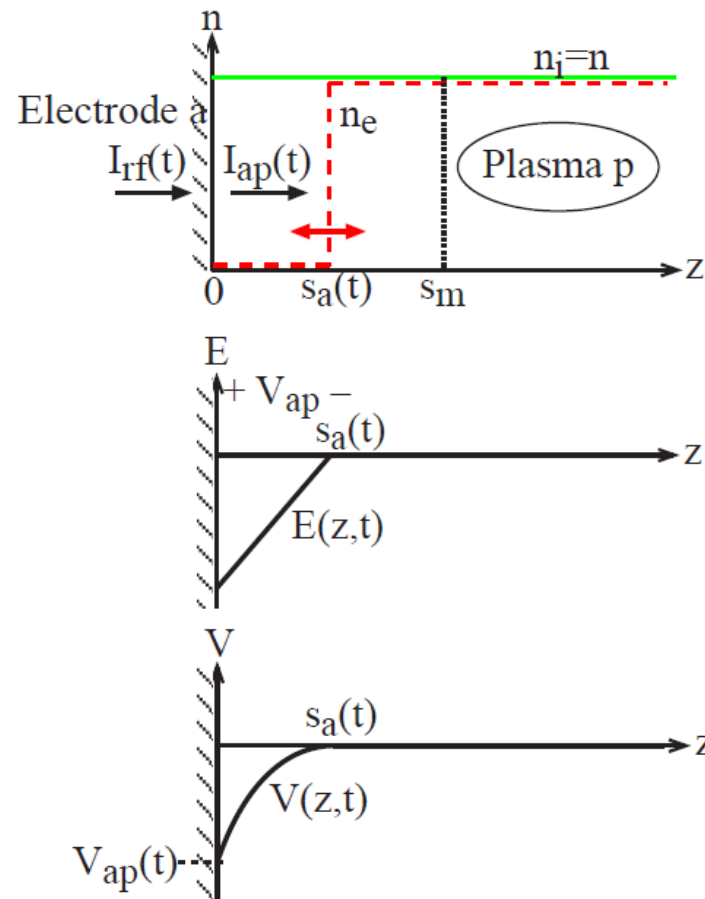
CONDUCTION CURRENT

- Assume a steady loss of ions to electrode a
$$I_i = enu_B A$$
- The time-average total conduction current to the electrode is zero
- Hence electrons must be lost to the electrode
- The sheath thickness $s_a(t)$ must then **collapse to zero** at some time during the rf cycle $\Rightarrow \bar{s}_0 = \tilde{s}_0$

$$s_a(t) = \tilde{s}_0(1 - \sin \omega t)$$



VOLTAGE ACROSS THE SHEATH



The voltage is found by integrating the electric field in the sheath

$$\frac{dV}{dz} = -E$$

VOLTAGE ACROSS THE SHEATH (CONT'D)

- Integrating the electric field in the sheath [p. 12]

$$\frac{dV}{dz} = -E$$

we obtain

$$V_{ap}(t) = \int_0^{s_a(t)} E(z, t) dz = -\frac{en}{\epsilon_0} \frac{s_a^2(t)}{2}$$

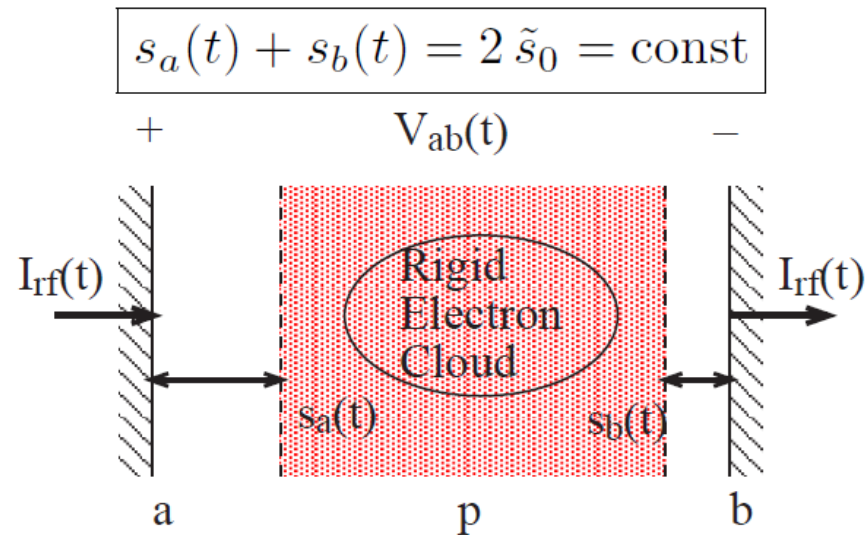
- Using $s_a(t)$ [p. 61]

$$V_{ap}(t) = -\frac{en}{2\epsilon_0} \tilde{s}_0^2 (1 - \sin \omega t)^2$$

- $V_{ap}(t)$ is a nonlinear function of I_{rf} ; there are second harmonics

VOLTAGE ACROSS BOTH SHEATHS

- By symmetry $s_b(t) = \tilde{s}_0(1 + \sin \omega t)$; since $s_a(t) = \tilde{s}_0(1 - \sin \omega t)$



- There is a **rigid bulk electron cloud oscillation**

VOLTAGE ACROSS BOTH SHEATHS (CONT'D)

- Voltage across sheath b is

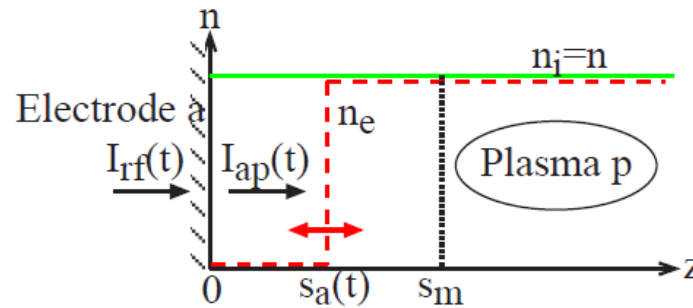
$$V_{bp}(t) = -\frac{en}{2\epsilon_0}\tilde{s}_0^2(1 + \sin \omega t)^2$$

- Voltage across the plasma is small because $I_{rf} = j\omega\epsilon_p EA$ and ϵ_p is large $\implies E$ across bulk plasma is small
- Discharge voltage is $V_{rf} = V_{ap} + V_{pb}$

$$V_{rf}(t) = \frac{2en\tilde{s}_0^2}{\epsilon_0} \sin \omega t$$

- Each sheath is nonlinear, but the combination of both sheaths is linear

DC VOLTAGE ACROSS ONE SHEATH



$$V_{pa}(t) = \frac{en}{2\epsilon_0} \tilde{s}_0^2 (1 - 2 \sin \omega t + \sin^2 \omega t)$$

- Take time average

$$\bar{V}_s = \frac{3}{4} \frac{en}{\epsilon_0} \tilde{s}_0^2 = \mathcal{E}_i$$

- Compare to rf voltage across discharge [p. 65]

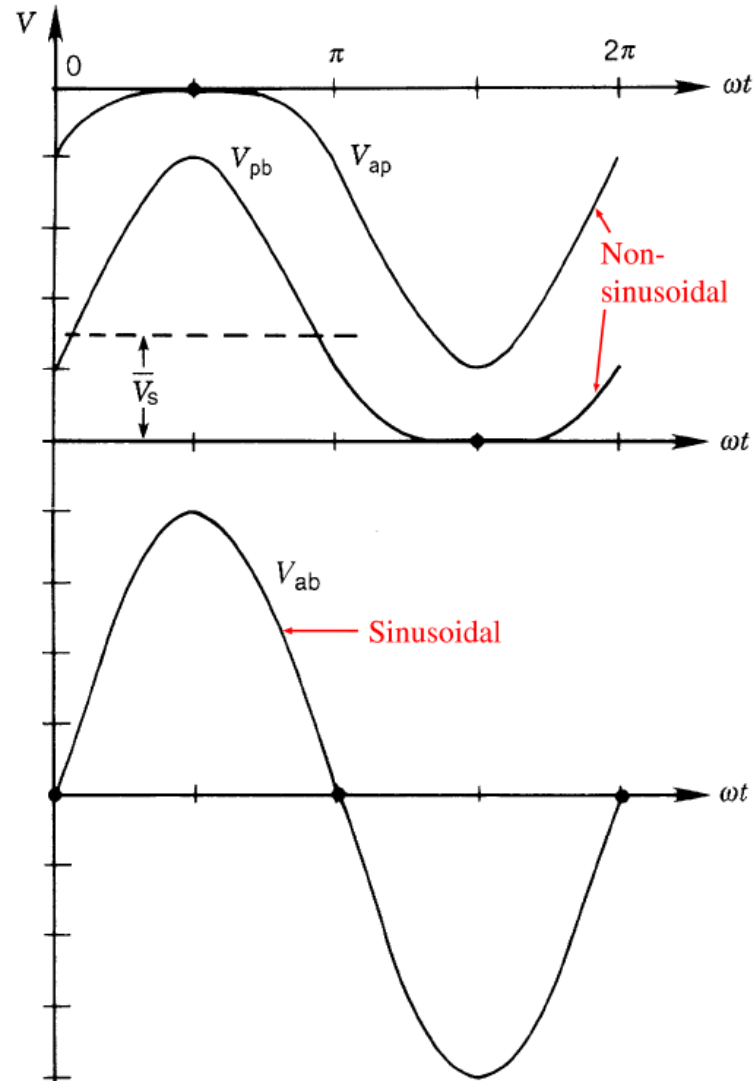
$$\Rightarrow \bar{V}_s = \frac{3}{8} \tilde{V}_{rf}$$

- We can think of \tilde{V}_{rf} as divided equally across the two sheaths

$$\bar{V}_s = \frac{3}{4} \tilde{V}_s \quad \text{with} \quad \tilde{V}_s = \frac{1}{2} V_{rf}$$

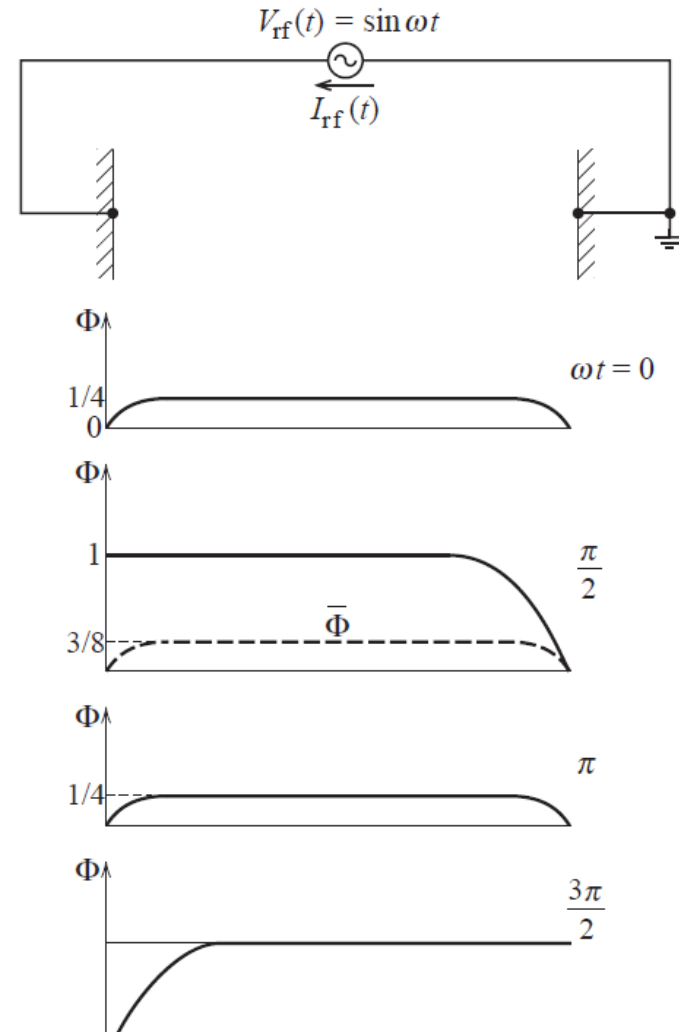
SHEATH VOLTAGES VERSUS TIME

Sheath voltages $V_{ap}(t)$, $V_{pb}(t)$, and their sum $V_{ab}(t) = V_{rf}(t)$; the time average \bar{V}_s of $V_{pb}(t)$ is also shown



SHEATH POTENTIAL VERSUS POSITION AT VARIOUS TIMES

Spatial variation of the total potential Φ (solid curves) for the homogeneous model at four different times during the rf cycle. The dashed curve shows the spatial variation of the time-average potential $\bar{\Phi} \equiv \bar{V}_s$



SHEATH CAPACITANCE

- Define total discharge capacitance by

$$I_{\text{rf}}(t) = \tilde{I}_0 \cos \omega t, \quad V_{\text{rf}}(t) = \frac{2en\tilde{s}_0^2}{\epsilon_0} \sin \omega t \quad [p. 65]$$

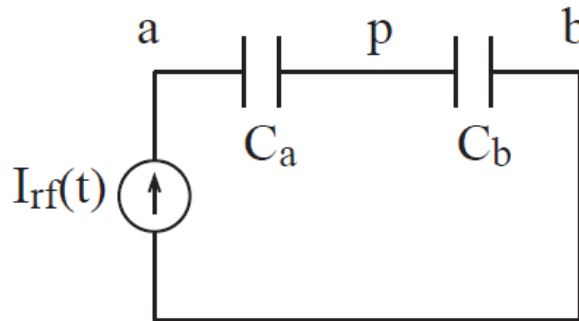
which yields

$$I_{\text{rf}} = C_s \frac{dV_{\text{rf}}}{dt} \quad \text{with} \quad C_s = \frac{\epsilon_0 A}{2\tilde{s}_0}$$

- We can think of each sheath as having a capacitance

$$C_a = C_b = \frac{\epsilon_0 A}{\tilde{s}_0}$$

- We now have a **lossless discharge model**

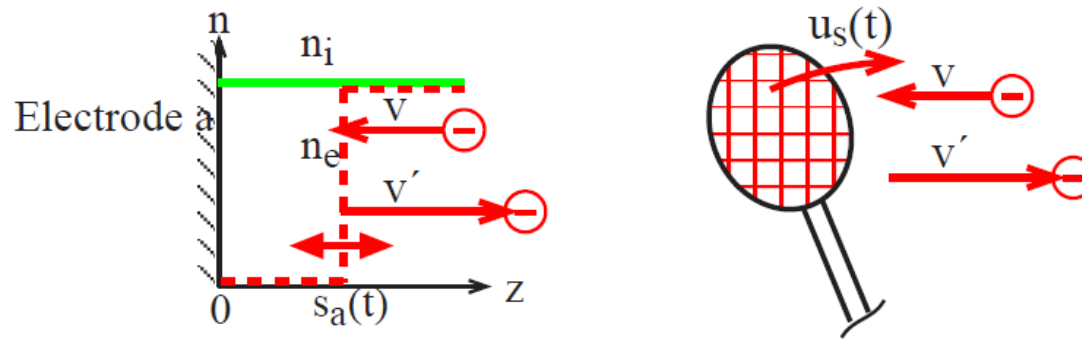


OHMIC AND STOCHASTIC HEATING

- Ohmic heating in the bulk plasma [p. 34]

$$P_{\Omega} = \frac{1}{2} |\tilde{J}_{\text{rf}}|^2 \frac{m \nu_m d}{e^2 n} A \quad [\text{watts}]$$

- Stochastic heating by oscillating sheaths



with

$$u_s(t) = \frac{ds_a}{dt} = \tilde{u}_0 \cos \omega t \quad \text{with} \quad \tilde{u}_0 = \omega \tilde{s}_0$$

- Average energy transferred is

$$\Delta \mathcal{E}_e = \left[\frac{1}{2} m (-v + 2u_s(t))^2 - \frac{1}{2} m v^2 \right] = m \tilde{u}_0^2$$

- $\Delta \mathcal{E}_e$ is positive, so the oscillating sheath heats electrons

STOCHASTIC HEATING POWER

- For a Maxwellian distribution, the electron flux incident on a sheath is [p. 17]

$$\Gamma_e = \frac{1}{4}n\bar{v}_e$$

with

$$\bar{v}_e = (8eT_e/\pi m)^{1/2}$$

the mean electron speed

- The time-average stochastic heating power is found to be

$$P_{sa} = \Gamma_e A \cdot 2 \Delta \mathcal{E}_e = \frac{1}{2} m n \bar{v}_e \omega^2 \tilde{s}_0^2 A \quad [\text{watts}]$$

- This is a **powerful electron heating mechanism** in a capacitive discharge

HEATING POWERS VERSUS DRIVING VOLTAGE

- For stochastic heating [p. 71]

$$P_{sa} = \frac{1}{2} m n \bar{v}_e \omega^2 \tilde{s}_0^2 A$$

Using $\tilde{V}_{\text{rf}} = 2en\tilde{s}_0^2/\epsilon_0$ [p. 65] we obtain for the two sheaths

$$P_s = P_{sa} + P_{sb} = \frac{m}{2e} \epsilon_0 \bar{v}_e \omega^2 \tilde{V}_{\text{rf}} A$$

- For bulk ohmic heating [p. 70]

$$P_{\Omega} = \frac{1}{2} |\tilde{J}_{\text{rf}}|^2 \frac{m \nu_m d}{e^2 n} A$$

Using $\tilde{J}_{\text{rf}} = en\omega\tilde{s}_0$ and \tilde{V}_{rf} given above

$$P_{\Omega} = \frac{m}{4e} \epsilon_0 \nu_m d \omega^2 \tilde{V}_{\text{rf}} A$$

Ohmic and stochastic heating powers depend on \tilde{V}_{rf}

Introduction to Plasma Simulation

Equations for neutral transport phenomena

Momentum conservation

$$\nabla \cdot (\rho_{mix} \vec{V} u_i) = -\frac{\partial P}{\partial x_i} + \nabla \cdot (\mu_{mix} \nabla u_i) + S_i$$

Mixed Viscosity by Kinetic theory

$$\mu_{mix} = f(\mu_i, x_i, \Phi_{ij}) \quad \leftarrow \quad \mu_i = f(\text{coefficient}, M_i, T, \sigma_i, \Omega_\mu)$$

Function of ()

Energy conservation

$$\nabla \cdot (\rho_{mix} \vec{V} h_0) = \nabla \cdot (k_{mix} \nabla T + P + \vec{\tau} \vec{V}) + S_h$$

$$h_0 = i + \frac{P}{\rho} + \frac{1}{2}(u^2 + v^2 + w^2)$$

h_0 : the total enthalpy

Mixed Conductivity by Kinetic theory

$$k_{mix} = f(k_i, x_i, \Phi_{ij}) \quad \leftarrow \quad k_i = f(\text{coefficient}, MW_i, C_{p,i}, R, \mu_i)$$

Mixed Molecular weight

$$MW_{mix} = \sum x_i M_i$$

Ideal gas

$$\rho_{mix} = \frac{(P + P_{ref}) MW_{mix}}{RT} \quad MW_{mix} : \text{Mixed Molecular weight}$$

Diffusivity by Kinetic theory

$$D_i = f(x_i, x_j, D_{ij}(M_{i_{or}j}, P, \Omega_D \sigma_{ij}))$$

$$D_i^T = f(x_i, x_j, T, D_{ij}(M_{i_{or}j}, P, \Omega_D \sigma_{ij}))$$

Species transport

$$\nabla \cdot (\rho_{mix} u_j Y_i) = \nabla \cdot \left(\Gamma \frac{\partial Y_i}{\partial x_j} \right) + (\dot{m}_k)_{evap}$$

$$Y_i = \sum \xi_{ik} f_k$$

f_k : The mixture fraction for the k mixture

Y_i : The mass fraction of species

ξ_{ik} : mass fraction of the I species in the k mixture

If Multi-component Diffusion

$$\Gamma \frac{\partial Y_i}{\partial x_j} = j_i \quad j_i = j_i^C + j_i^T \quad j_i^C = -\rho D_i^C \nabla Y_i : \text{concentration-driven diffusion}$$

$$j_i^T = -\rho D_i^T \nabla (\ln T) : \text{Thermo-diffusion or soret diffusion}$$

μ_i : Viscosity of species i

T : Temperature

M_i : Molecular weight of species i

x_i : Mole fraction of species i

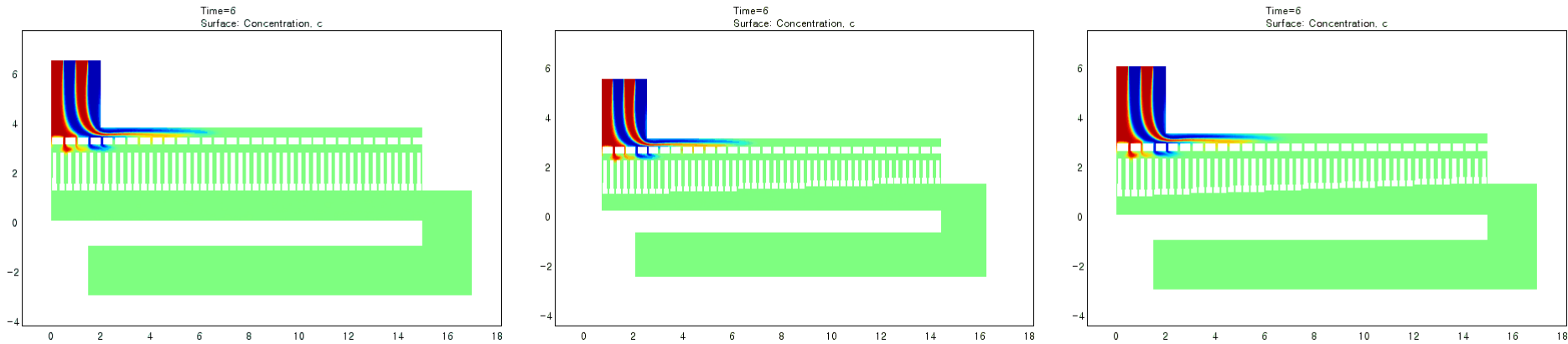
σ_i : Lennard-Jones collision diameter

Ω : collision integral

Φ_{ij} : dimensionless quantity

-> function of Molecular weight

Importance of careful consideration of diffusion



- Scalar fields are described by convection, diffusion and reaction.
- Convection → important in a transient problem, odd-order error, wave propagation
- Diffusion → important in a steady problem, even-order error, artificial diffusion
- In a vacuum system (i.e., $P_{\text{op}} < 200$ Torr), reactor is under the diffusion dominating condition because Re is low.
- In an RF discharge problem, if the system is assumed as a continuum regime, normally thermal velocity is much larger than electron velocity. Thus inertia term can be neglected, and we can use “drift-diffusion approximation”. This drift-diffusion approximation makes electron energy equation diffusion dominating.
- Thus accurate solving for diffusion term is critical to simulate semiconductor fabrication system.

Transport of neutral species (stable molecules, radicals, ...)

$$\frac{\partial}{\partial t}(\rho Y_i) = -\nabla \cdot (\rho \mathbf{v} Y_i) - \nabla \cdot (j_i^C + j_i^T) + (G_i - L_i) M_i$$

ρ - the overall density

\mathbf{v} - the overall velocity

Y_i - the mass fraction of species i

j_i^C - the flux of species i due to the concentration gradients

j_i^T - the thermal diffusion flux of species i

G_i - the generation rate of species i

L_i - the depletion rate of species i

M_i - the molar mass of species i

Equations for charged species (Fluid model)

$$\frac{\partial n_p}{\partial t} + \nabla \cdot (n_p \mathbf{v}_p) = n_e N k_i$$

positive ion continuity

$$n_p \mathbf{v}_p = n_p \mu_p \mathbf{E} - D_p \nabla n_p$$

drift-diffusion approximation

$$\frac{\partial n_n}{\partial t} + \nabla \cdot (n_n \mathbf{v}_n) = n_e N k_i$$

negative ion continuity

$$n_n \mathbf{v}_n = n_n \mu_n \mathbf{E} - D_n \nabla n_n$$

drift-diffusion approximation

$$\frac{\partial n_e}{\partial t} + \nabla \cdot (n_e \mathbf{v}_e) = n_e N k_i$$

electron continuity

$$n_e \mathbf{v}_e = -n_e \mu_e \mathbf{E} - D_e \nabla n_e$$

drift-diffusion approximation

Continuity Equation

$$\frac{\partial n_e \varepsilon_e}{\partial t} + \nabla \cdot \left(\frac{5}{3} n_e \varepsilon_e \mathbf{v}_e + \mathbf{q}_e \right) = -e n_e \mathbf{v}_e \cdot \mathbf{E} - n_e N k_L$$

$$\mathbf{q}_e = -\frac{2}{3} \kappa \nabla \varepsilon_e$$

$$\kappa = \frac{5}{2} n_e D_e$$

D_e eventually governs the dissociation rate profile in the gas phase.

If the gas phase reaction is more active than surface reaction, deposition profile will be a function of N_e distribution.

$$\mathbf{E} = -\nabla V$$

Electron Energy Equation

$$\Delta V = -\frac{e}{\varepsilon_0} (n_p - n_n - n_e)$$

Poisson equation

Surface phenomena: sticking model & molecular dynamics

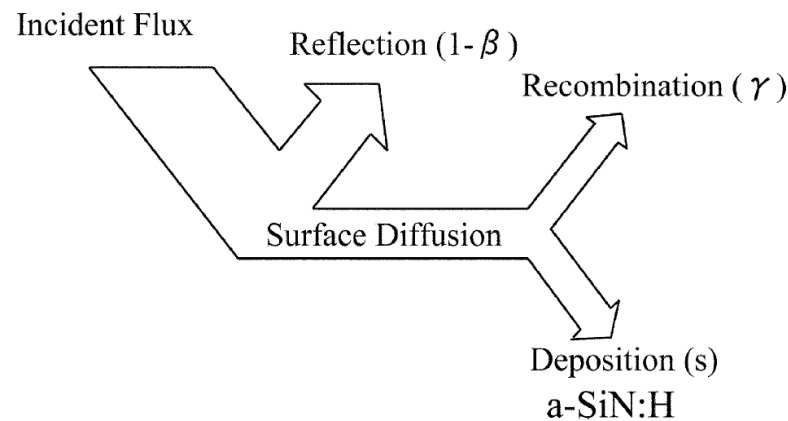
Deposition by radical species can be described by utilization of a phenomenological approach called as a sticking model.

$$-D_i \frac{\partial n_i}{\partial z} = -R_{i,s}(n_{i,s}) = \Gamma_i^{in} + \Gamma_i^{out}$$

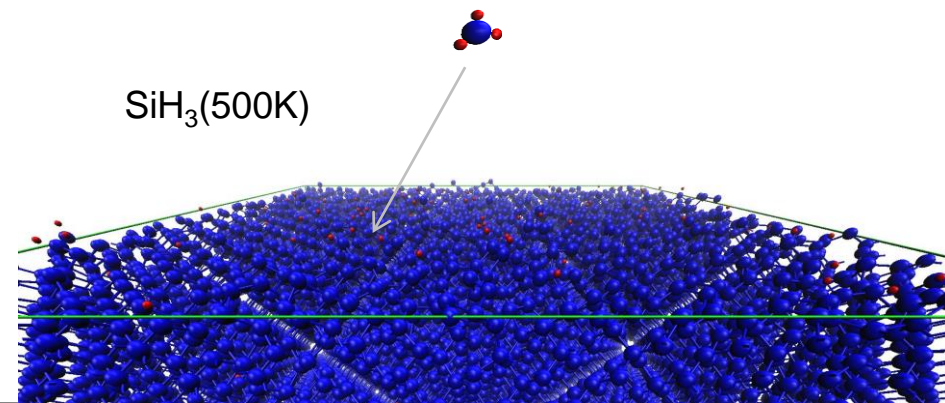
$$\Gamma_i^{in} = \frac{s_i + \gamma_i}{1 - (s_i + \gamma_i)/2} n_{i,s} \sqrt{\frac{k_B T_g}{2\pi m_i}}$$

$$\Gamma_i^{out} = -\sum_{j \neq i} \frac{\gamma_j}{s_j + \gamma_j} \Gamma_j^{in}$$

where subscript i , D_i , n_i , z , $n_{i,s}$, and $R_{i,s}$ are the species index, the diffusion coefficient, the density of species i , the axial coordinate, the density of species i at the surface, and the surface reaction rate of species i , respectively.

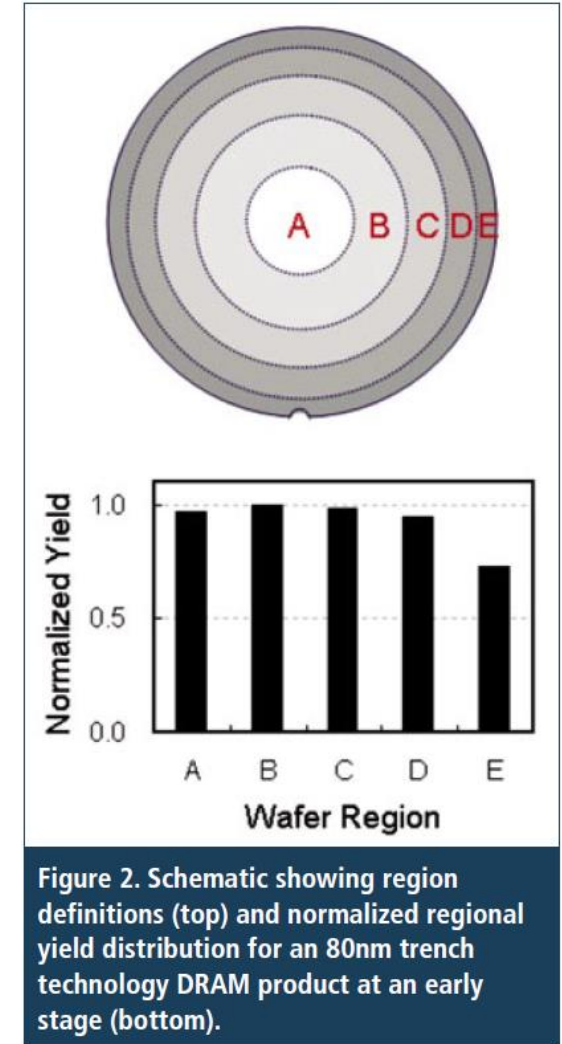
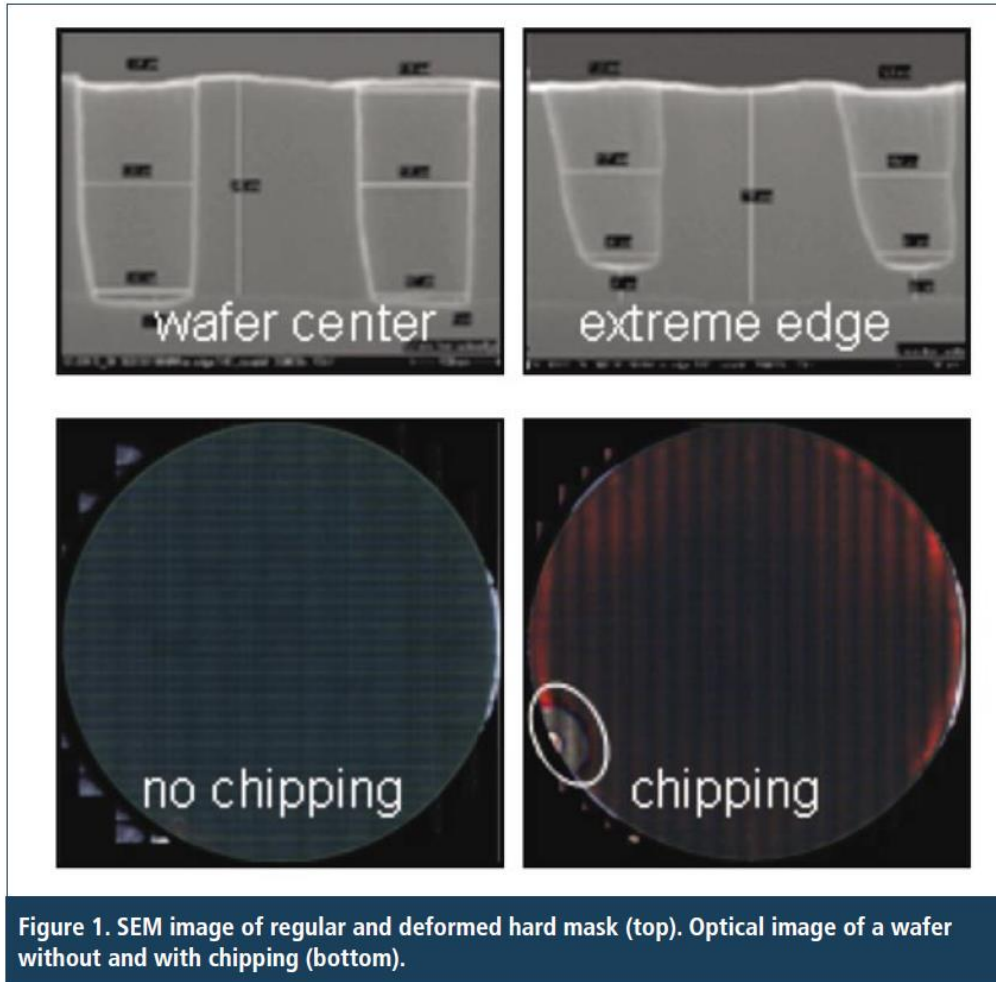


Molecular Dynamics Simulations (s , β , γ)



Case Studies

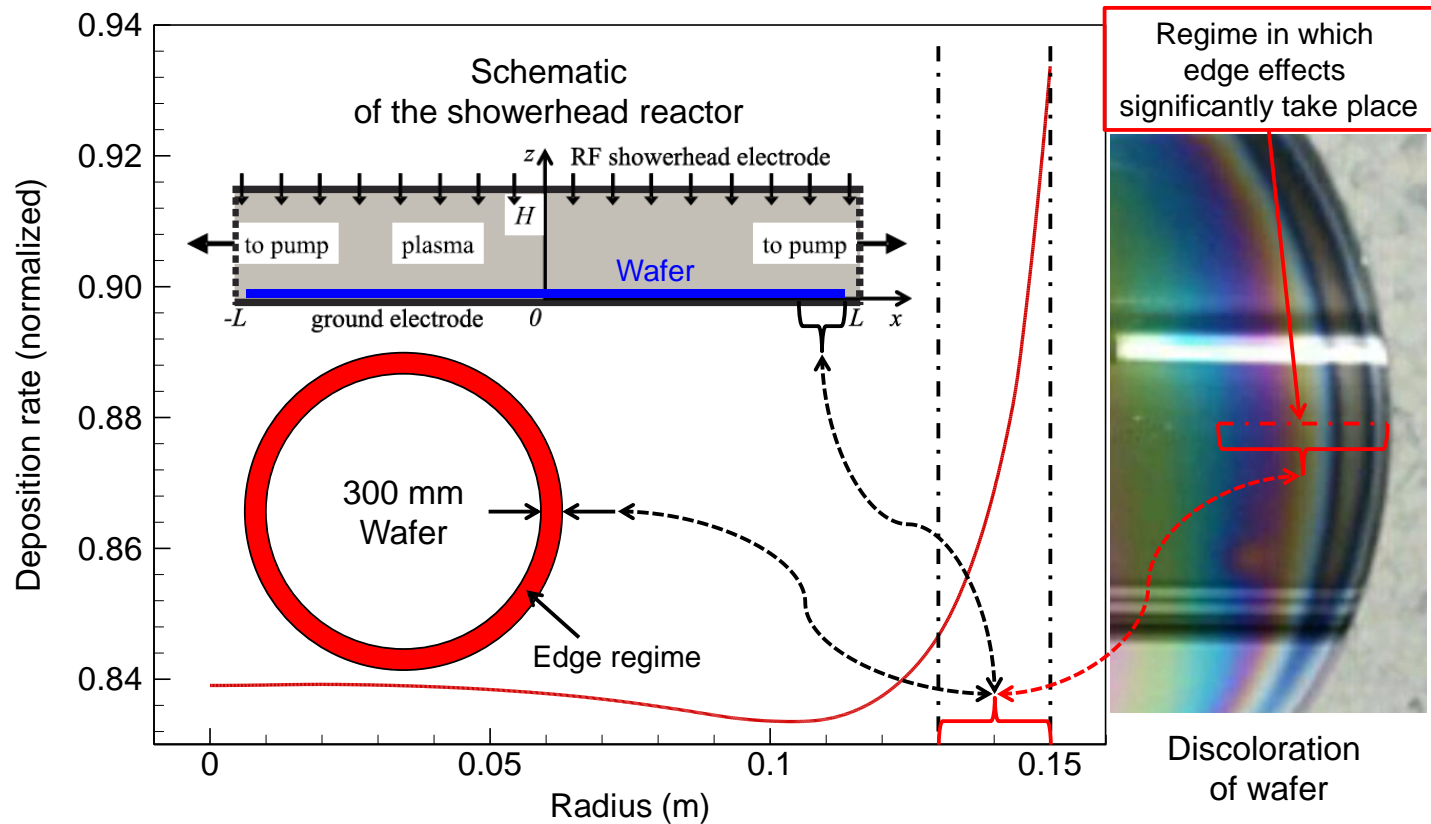
Non-uniformity issues observed in the wafer edge



Source: *Wafer-edge yield engineering in leading-edge DRAM manufacturing* by Oguz Yavas, Ernst Richter, Christian Kluthe & Markus Sickmoeller, Qimonda AG

Non-uniformity issues observed in the wafer edge

Ho Jun Kim and Hae June Lee **2017** Effects of the wall boundary conditions of a showerhead plasma reactor on the uniformity control of RF plasma deposition *Journal of Applied Physics* **122** 053301

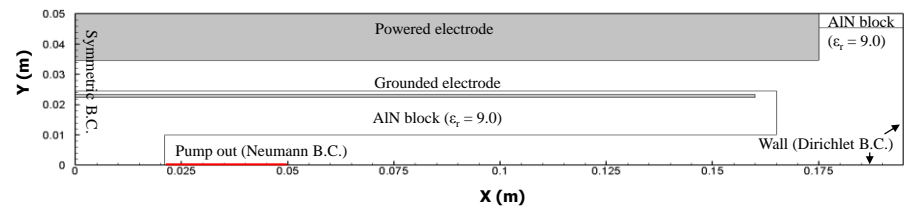


For a typical case with nonuniformity in the edge thickness, its deposition rate profile is plotted along the electrode radius ($0 \leq r \leq 150$ mm, where r is the radial coordinate) with a solid red line. Near the edge ($r \geq 120$ mm), the deposition rate varies greatly, and concomitantly the corresponding area of wafer shows discoloration (see inset). As shown in the schematic of the showerhead reactor, the geometric configuration of a reactor can give rise to significant spatial changes in various physical aspects.

Plasma reactor simulation: Capacitively Coupled Plasma

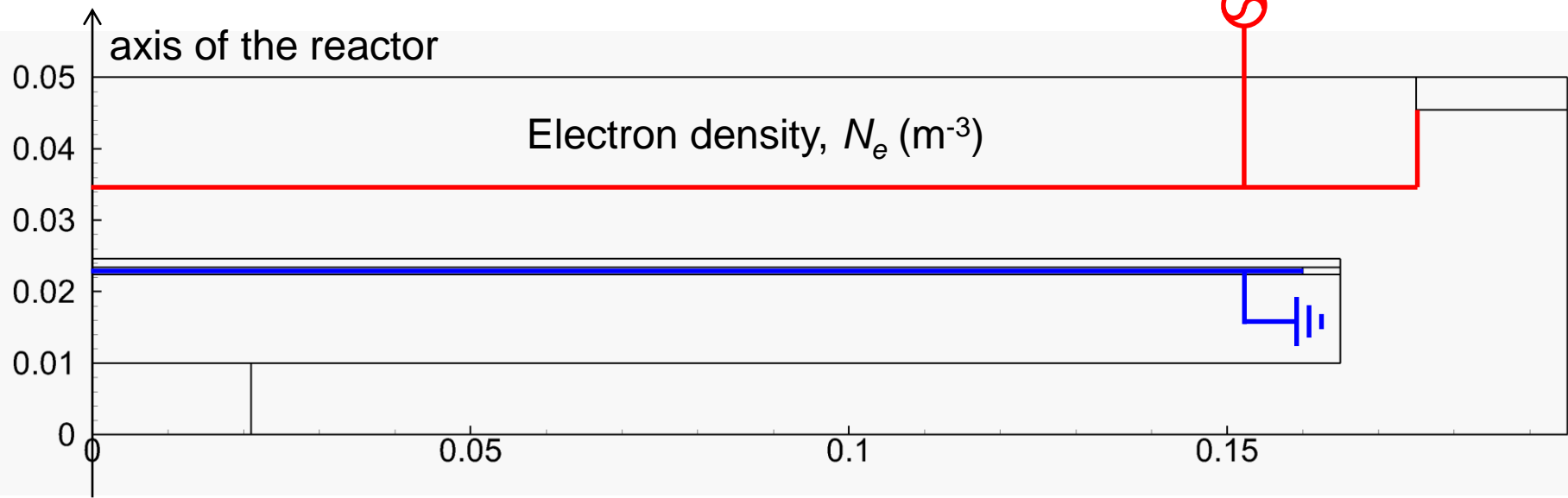
Domain for simulation

❖ Domain



Normally, the reactor is Cylindrical → due to a wafer shape
Axi-symmetric

The off-axis maximum of the electron density is observed!



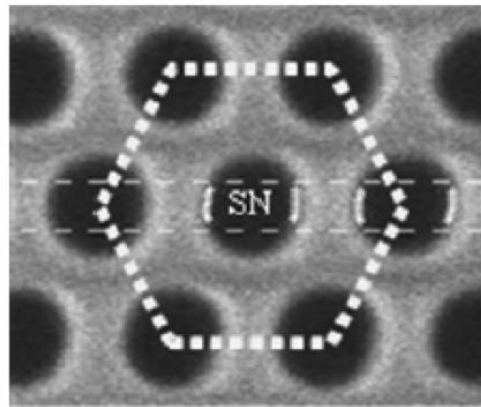
PIC simulation from Kim *et al.* of PNU



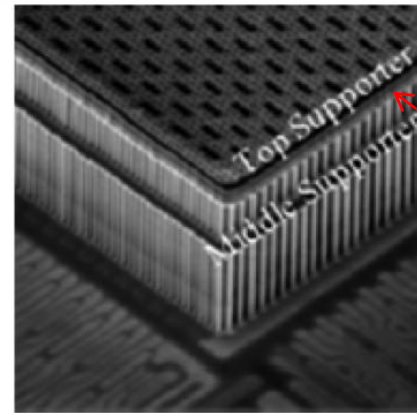
Application:

SiN_xH_y layer deposition
a-Si:H layer deposition

SiN_xH_y film utilized in the memory fabrication



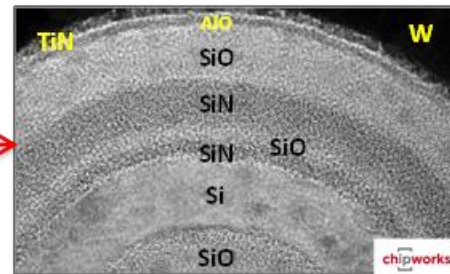
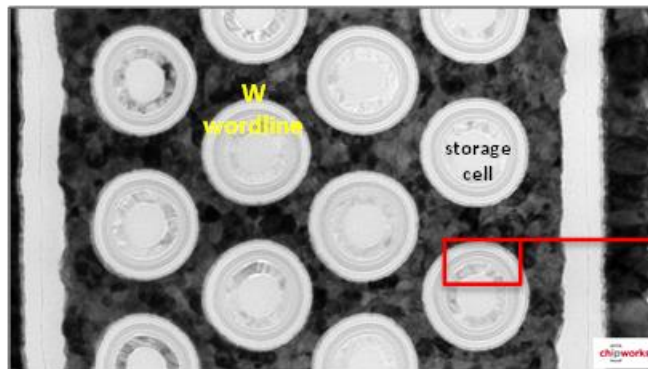
(a) A Plane view of honeycomb structure



(b) A birds' eye view of honeycomb

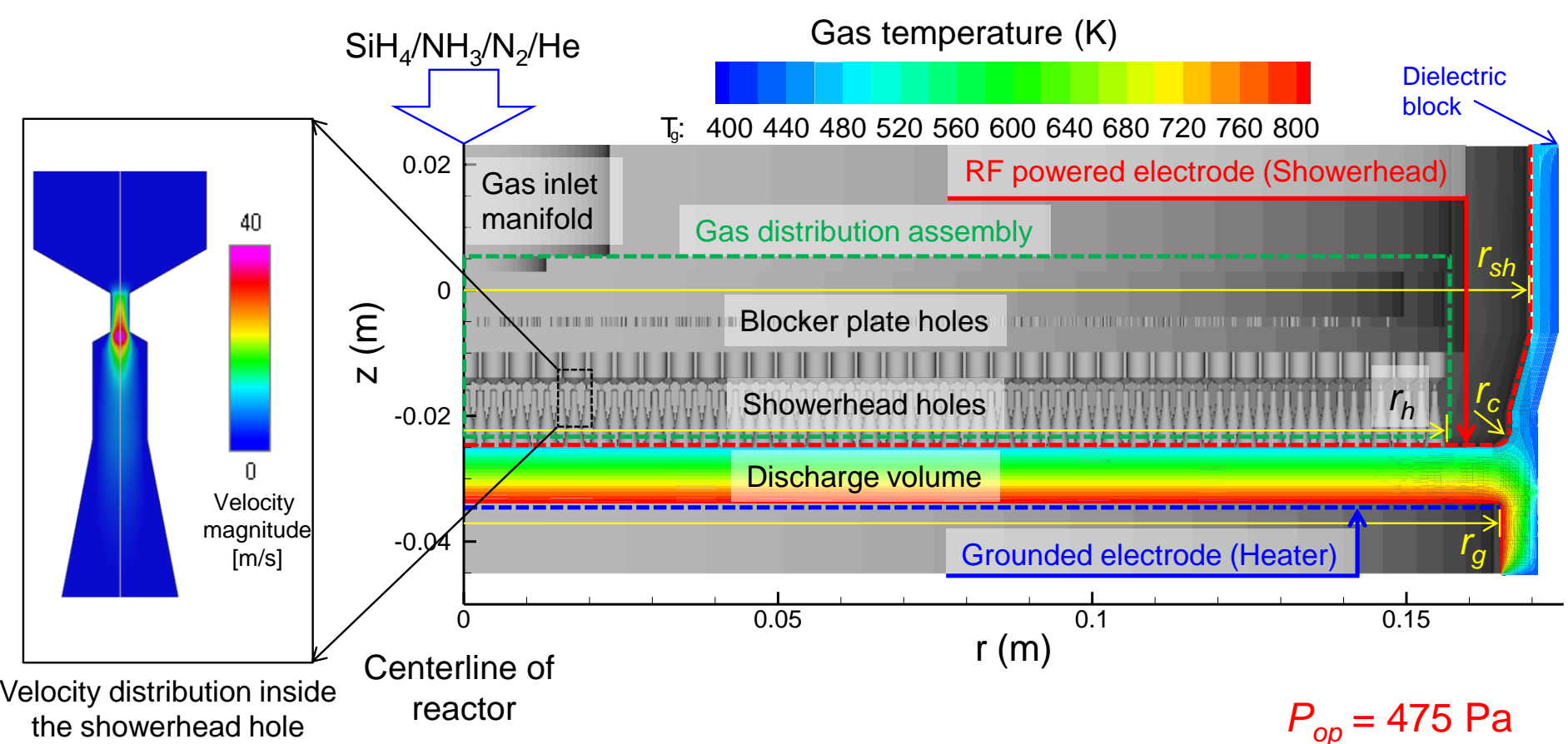
SiN_xH_y film

Pan-view images of Samsung 20 nm DRAM



Plan-view images of Samsung V-NAND flash array

Reactor configuration used for SiN_xH_y deposition

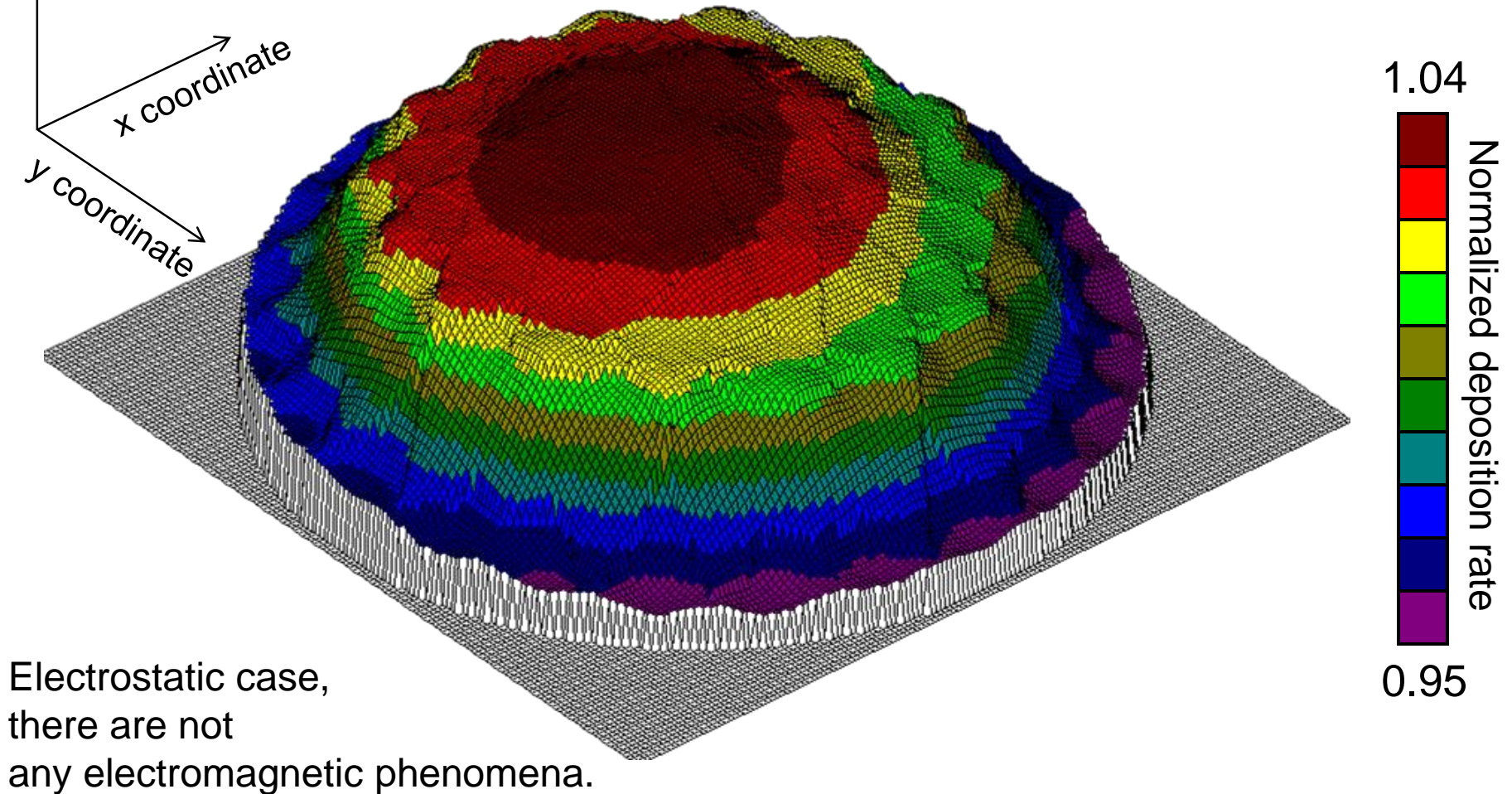


CCP reactor configuration is plotted together with the spatial variation of the gas temperature. The inset shows the velocity distribution obtained by a numerical simulation of neutral gas flow in the showerhead hole. The reactor dimensions are also depicted.

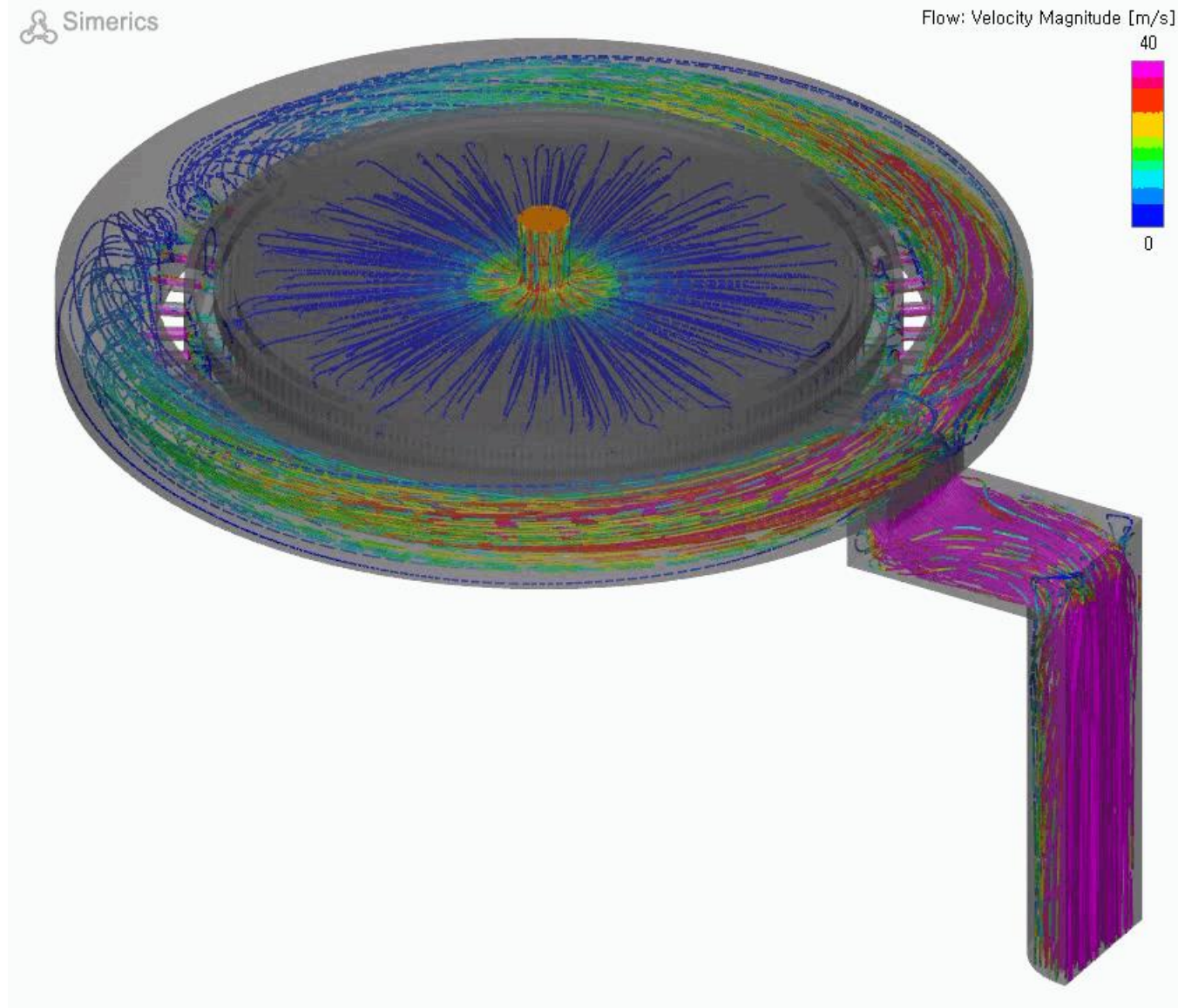
Deposition rate contour experimentally measured

Deposition rate
x coordinate
y coordinate

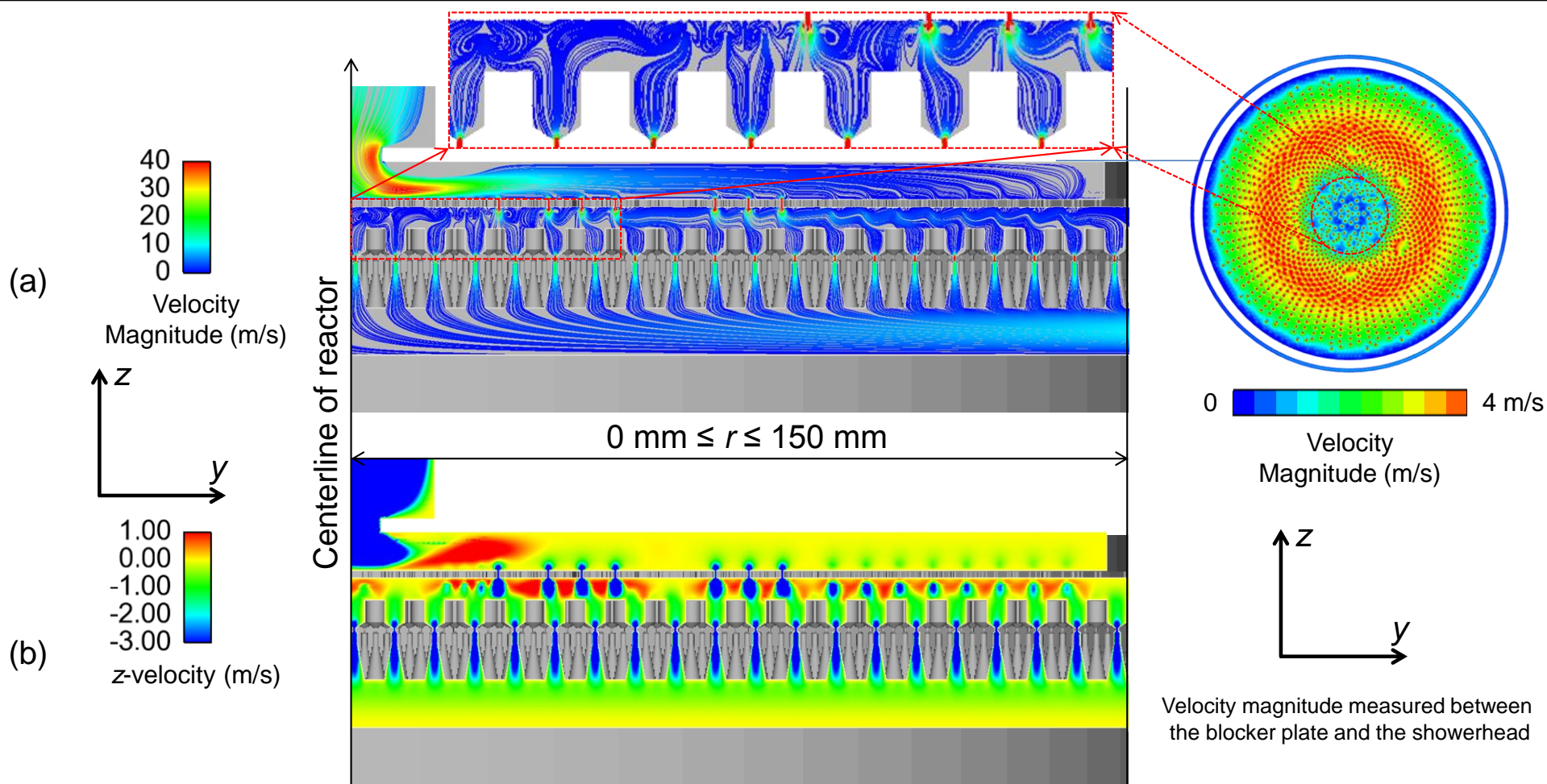
In the center of the deposition rate contour, non-negligible variation can be observed.



Gas flow simulation performed with a realistic 3D geometry

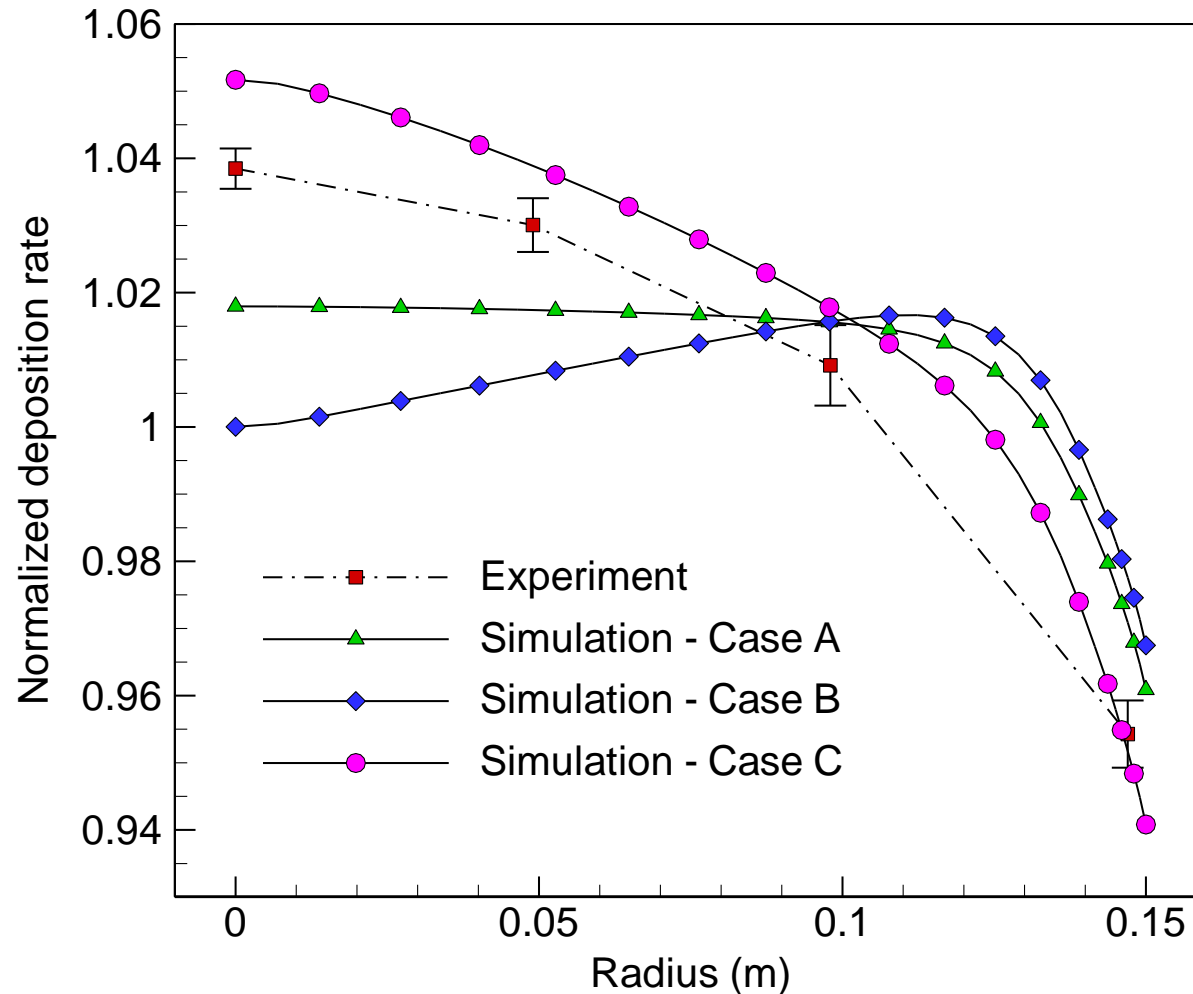


Gas flow simulation performed with a realistic 3D geometry



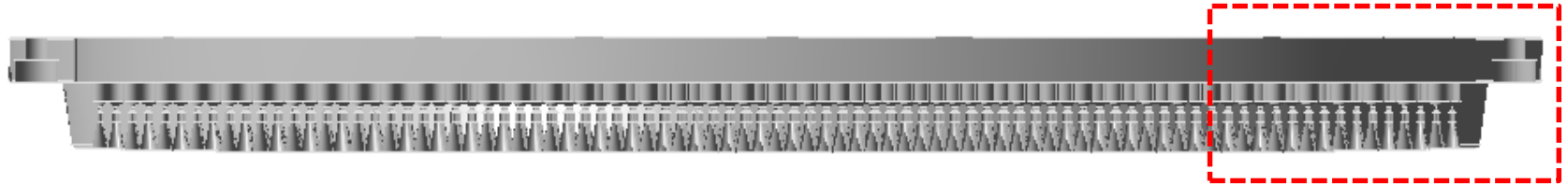
Results of the 3D gas flow simulation: (a) streamlines and velocity magnitude and (b) z-velocity contour plot. In the inset of (a), it is observed that the streamlines of the interim space between the blocker plate and showerhead are most curled at the center of the reactor ($r \leq 50 \text{ mm}$).

Validation: deposition rate profiles

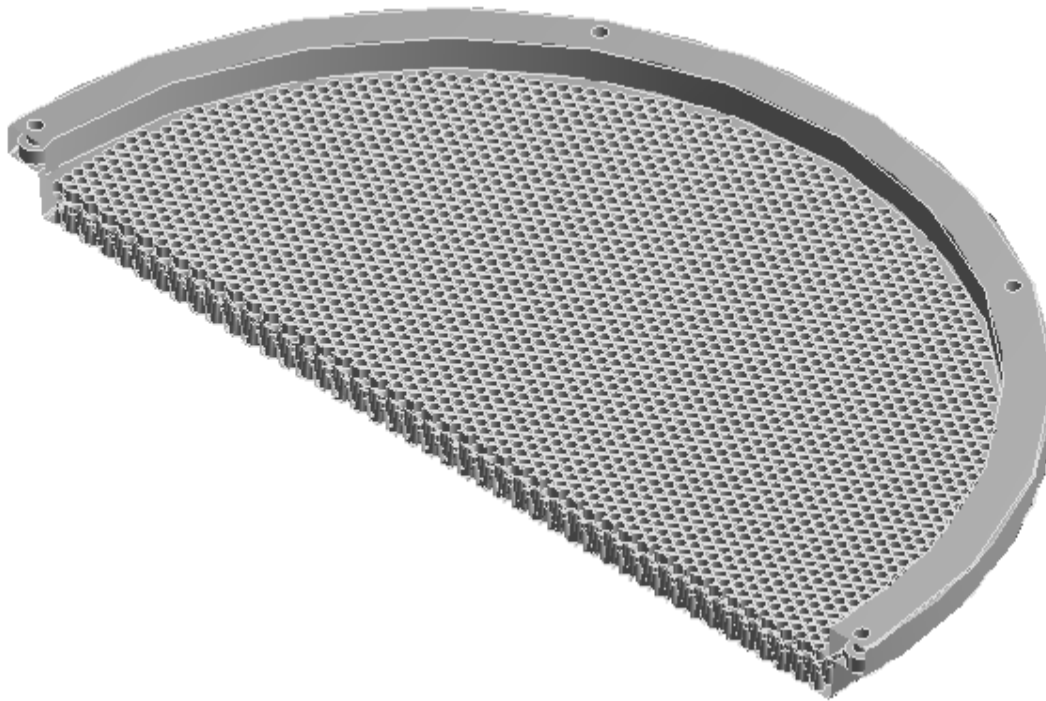


The simulated deposition rates along the wafer radius are depicted for the three different profiles of inlet gas density at the showerhead and compared with the experimental results.

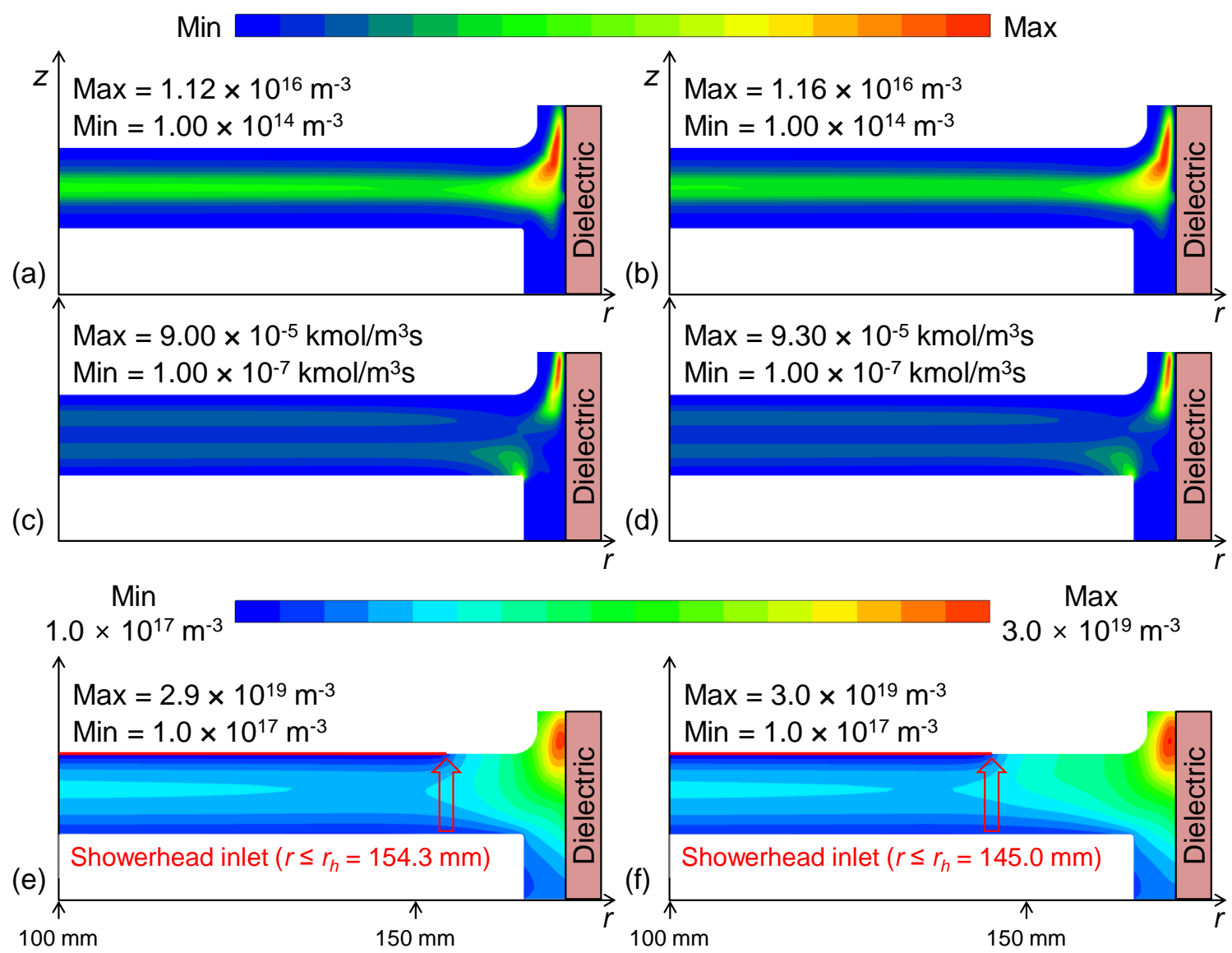
Showerhead analysis



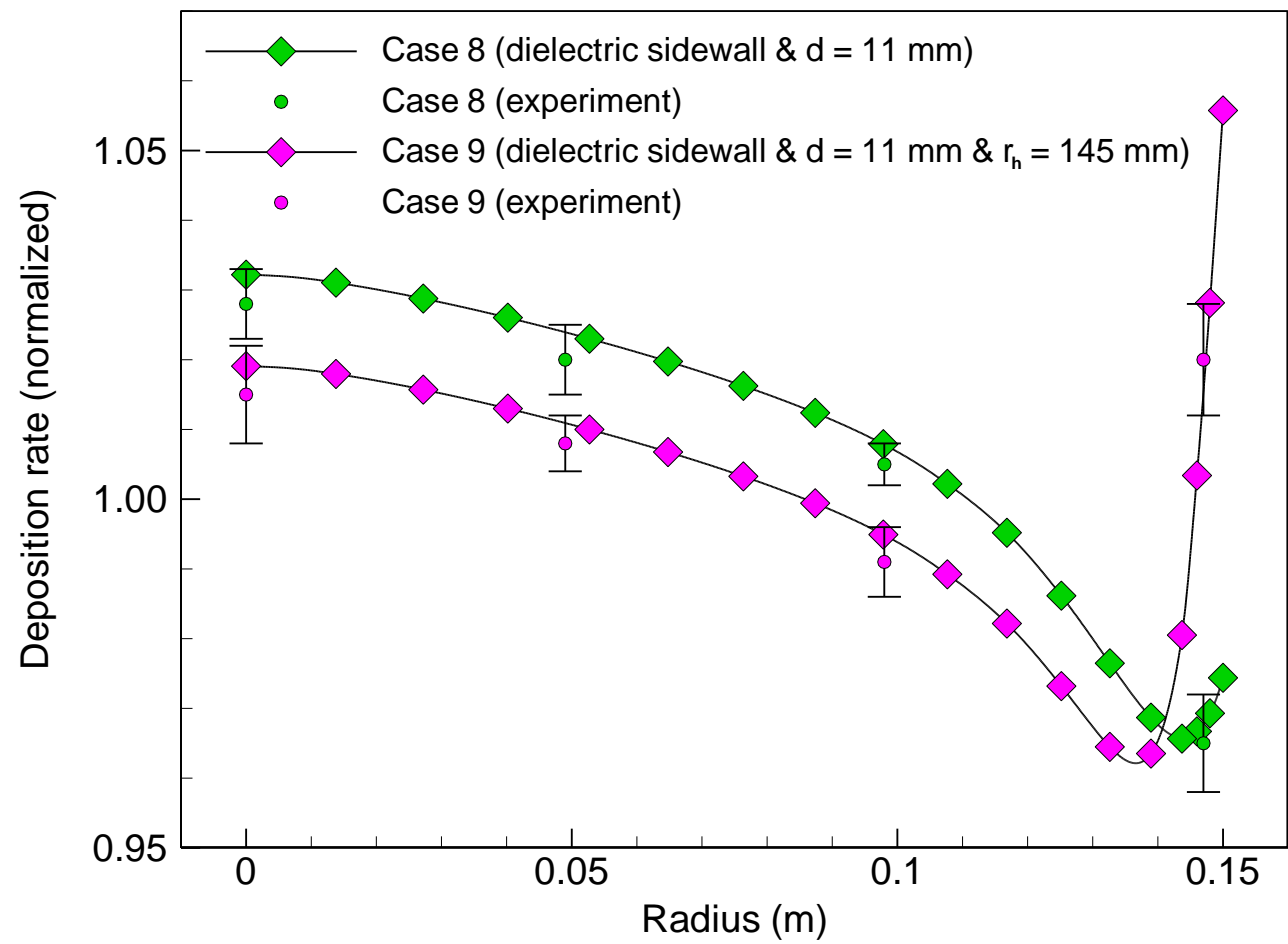
block



Effects of the shower radius



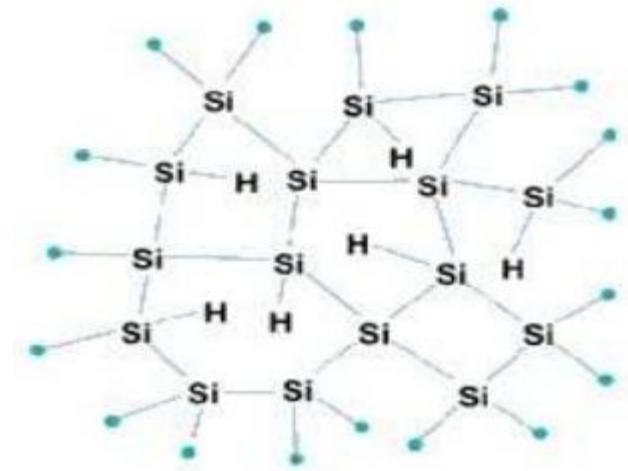
Effects of the shower radius



The deposition rate profiles of experimental measurement agree well with the simulation results for the variation of shower radius, with $r_h = 154.3$ mm (case 8) and $r_h = 145$ mm (case 9). The increased N density near the electrode radius induces an increase of the deposition rate profile near the edge for the case with $r_h = 145$ mm.

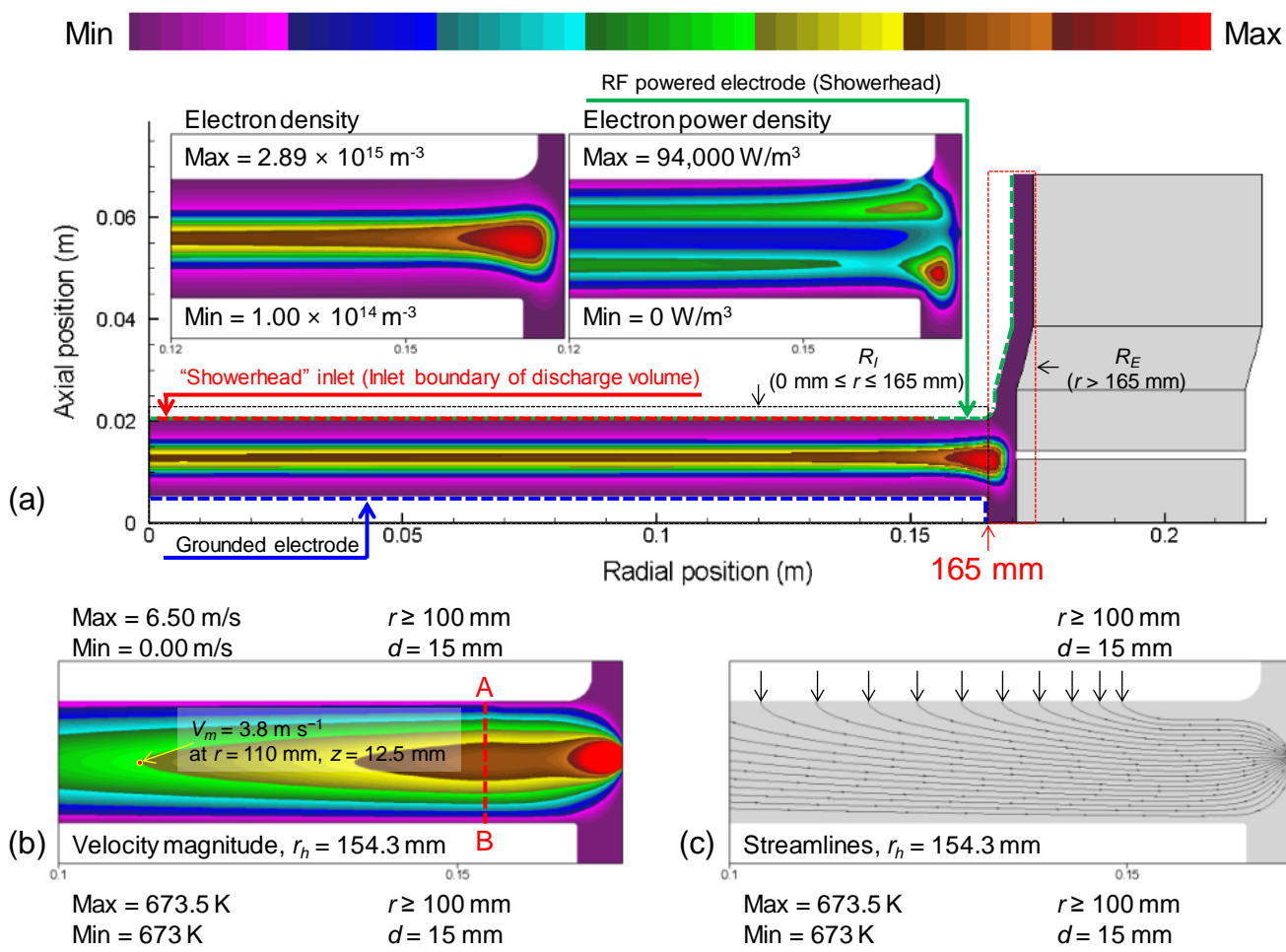
Hydrogenated amorphous silicon: a-Si:H

- The term “amorphous” commonly applied to non-crystalline materials prepared by deposition from gases. In amorphous silicon the long range order is not present. Rather, the atoms form a continuous random networks.
- The electronic-grade amorphous silicon is called hydrogenated amorphous silicon (a-Si:H). It is also an alloy of silicon and hydrogen.
- In early studies of amorphous silicon, it was determined that plasma-deposited amorphous silicon contained a significant percentage of hydrogen atoms bonded into the amorphous silicon structure.
- These atoms were discovered to be essential to the improvement of the electronic properties of the material.



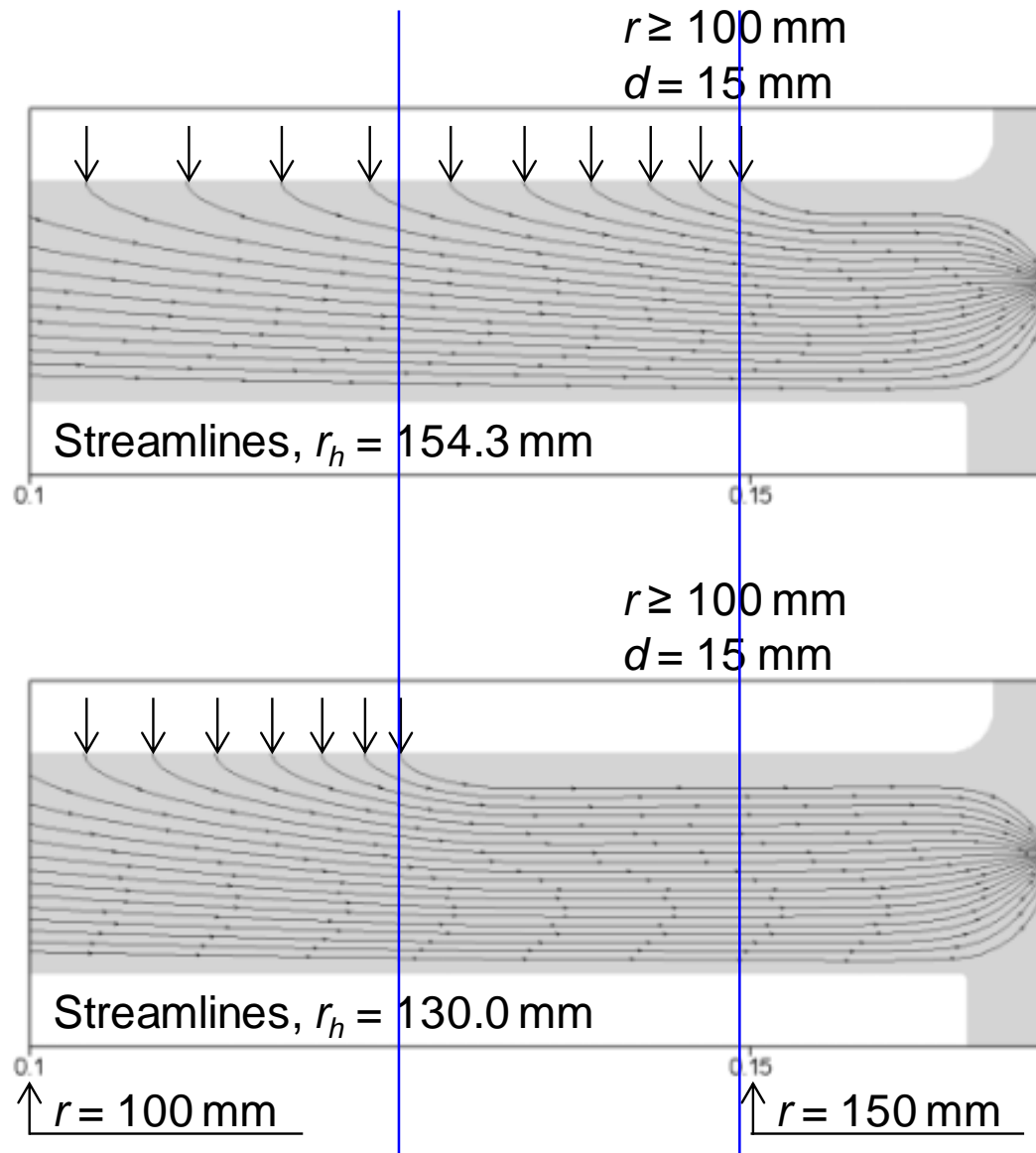
a-Si:H Structure

Reactor configuration used for a-Si:H deposition



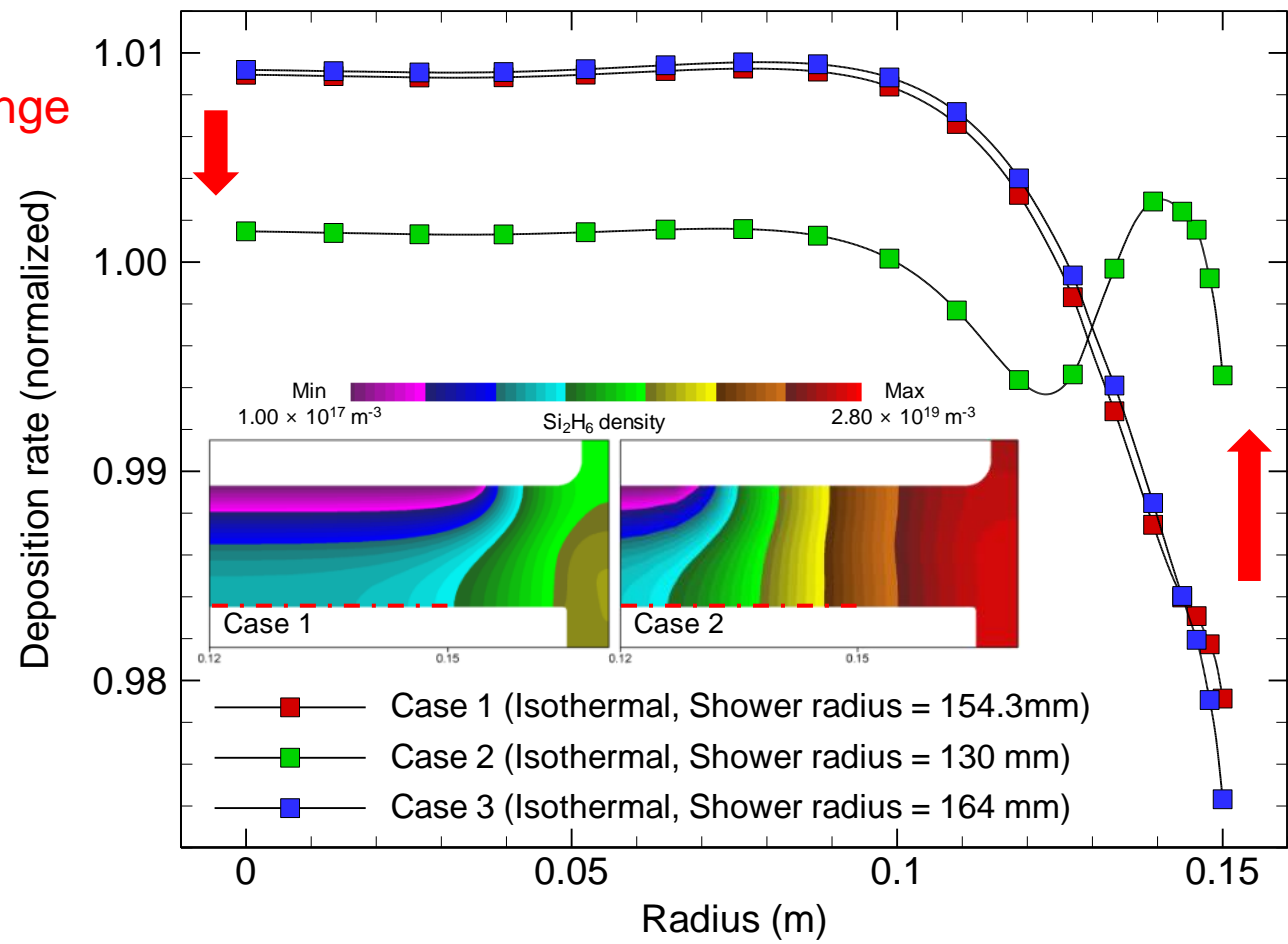
Schematic diagram of a cylindrically symmetric showerhead reactor. Because of its geometric axisymmetry, only half of the reactor is shown. The left boundary denotes the axis of symmetry, and the right boundary denotes the radial wall (i.e., the sidewall). The spatial variations in (a) electron density, N_e (m^{-3}) and (b) velocity magnitude, V_m (m s^{-1}), are depicted for the base case (Case 1). In the inset of (a), the spatial variation of time-averaged electron power density, P_e (W m^{-3}), is also depicted. (c) The streamlines are drawn in black.

Effects of the gas distribution



Effects of the gas distribution

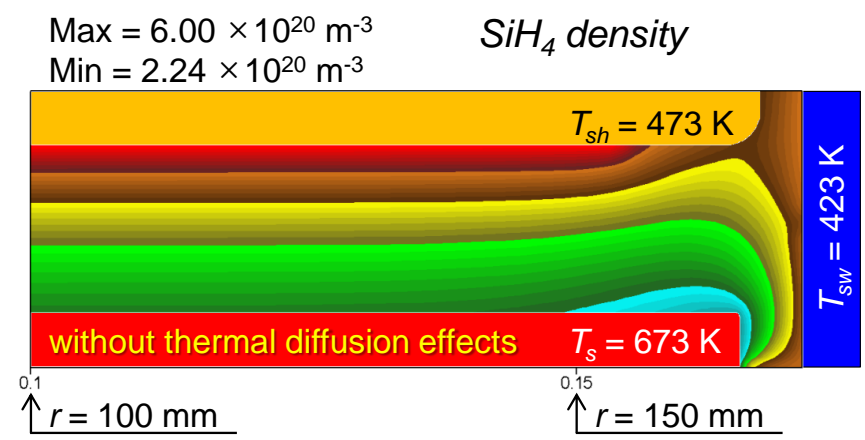
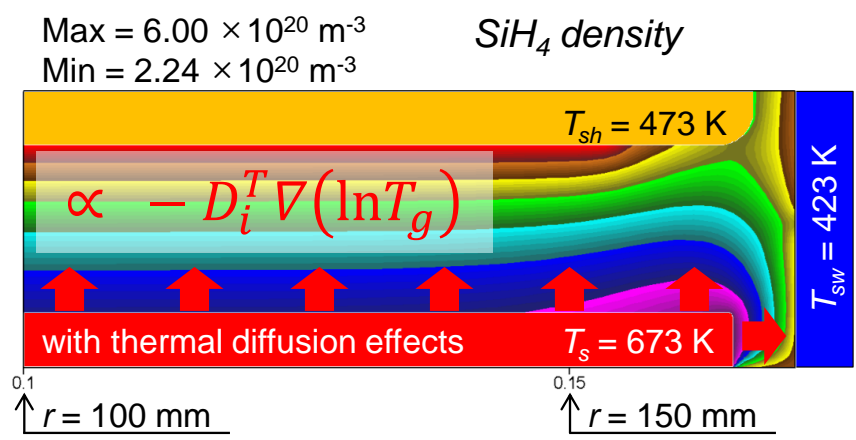
Simple change
makes
the big
difference !



Simulated deposition rates measured along the radial direction for Cases 1 (red square), 2 (green square), and 3 (blue square). The rates are normalized to their corresponding averaged values. In the inset, the spatial variations of Si_2H_6 densities are depicted for Cases 1 and 2.



Effects of the thermal diffusion



$$j_i^T = -D_i^T \nabla(\ln T_g)$$

$$D_i^T = \alpha D_i M_i M_j c_g^2 / \rho_g$$

$$\alpha = \frac{1}{6\lambda_{ij}} \left(\frac{S^{(i)} f_i - S^{(j)} f_j}{X_\lambda + Y_\lambda} \right) (6C_{ij}^* - 5)$$

$$S^{(i)} = \left(\frac{M_i + M_j}{2M_j} \right) \frac{\lambda_{ij}}{\lambda_i} - \frac{15}{4A_{ij}^*} \left(\frac{M_j - M_i}{2M_i} \right) - 1$$

$$S^{(j)} = \left(\frac{M_j + M_i}{2M_i} \right) \frac{\lambda_{ij}}{\lambda_j} - \frac{15}{4A_{ij}^*} \left(\frac{M_i - M_j}{2M_j} \right) - 1$$

$$X_\lambda = \frac{f_i^2}{\lambda_i} + \frac{2f_i f_j}{\lambda_{ij}} + \frac{f_j^2}{\lambda_j}$$

$$Y_\lambda = \frac{f_i^2}{\lambda_i} U^{(i)} + \frac{2f_i f_j}{\lambda_{ij}} U^{(Y)} + \frac{f_j^2}{\lambda_j} U^{(j)}$$

$$U^{(i)} = \frac{4}{15} A_{ij}^* - \frac{1}{12} \left(\frac{12}{5} B_{ij}^* + 1 \right) \frac{M_i}{M_j} + \frac{1}{2} \frac{(M_i - M_j)^2}{M_i M_j}$$

$$U^{(j)} = \frac{4}{15} A_{ij}^* - \frac{1}{12} \left(\frac{12}{5} B_{ij}^* + 1 \right) \frac{M_j}{M_i} + \frac{1}{2} \frac{(M_j - M_i)^2}{M_i M_j}$$

$$U^{(Y)} = \frac{4}{15} A_{ij}^* \left(\frac{(M_i + M_j)^2}{4M_i M_j} \right) \frac{\lambda_{ij}^2}{\lambda_i \lambda_j} - \frac{1}{12} \left(\frac{12}{5} B_{ij}^* + 1 \right) - \frac{5}{32 A_{ij}^*} \left(\frac{12}{5} B_{ij}^* - 5 \right) \frac{(M_i - M_j)^2}{M_i M_j}$$

$$\lambda_i = 8.32 \times 10^{-4} \frac{(T_g / M_i)^{1/2}}{\sigma_i^2 \Omega_i^{(2,2)*}}$$

$$\lambda_{ij} = 8.32 \times 10^{-4} \frac{[T_g (M_i + M_j) / 2M_i M_j]^{1/2}}{\sigma_{ij}^2 \Omega_{ij}^{(2,2)*}}$$

$$A_{ij}^* = \Omega_{ij}^{(2,2)*} / \Omega_{ij}^{(1,1)*}$$

$$B_{ij}^* = [5\Omega_{ij}^{(1,2)*} - 4\Omega_{ij}^{(1,3)*}] / \Omega_{ij}^{(1,1)*}$$

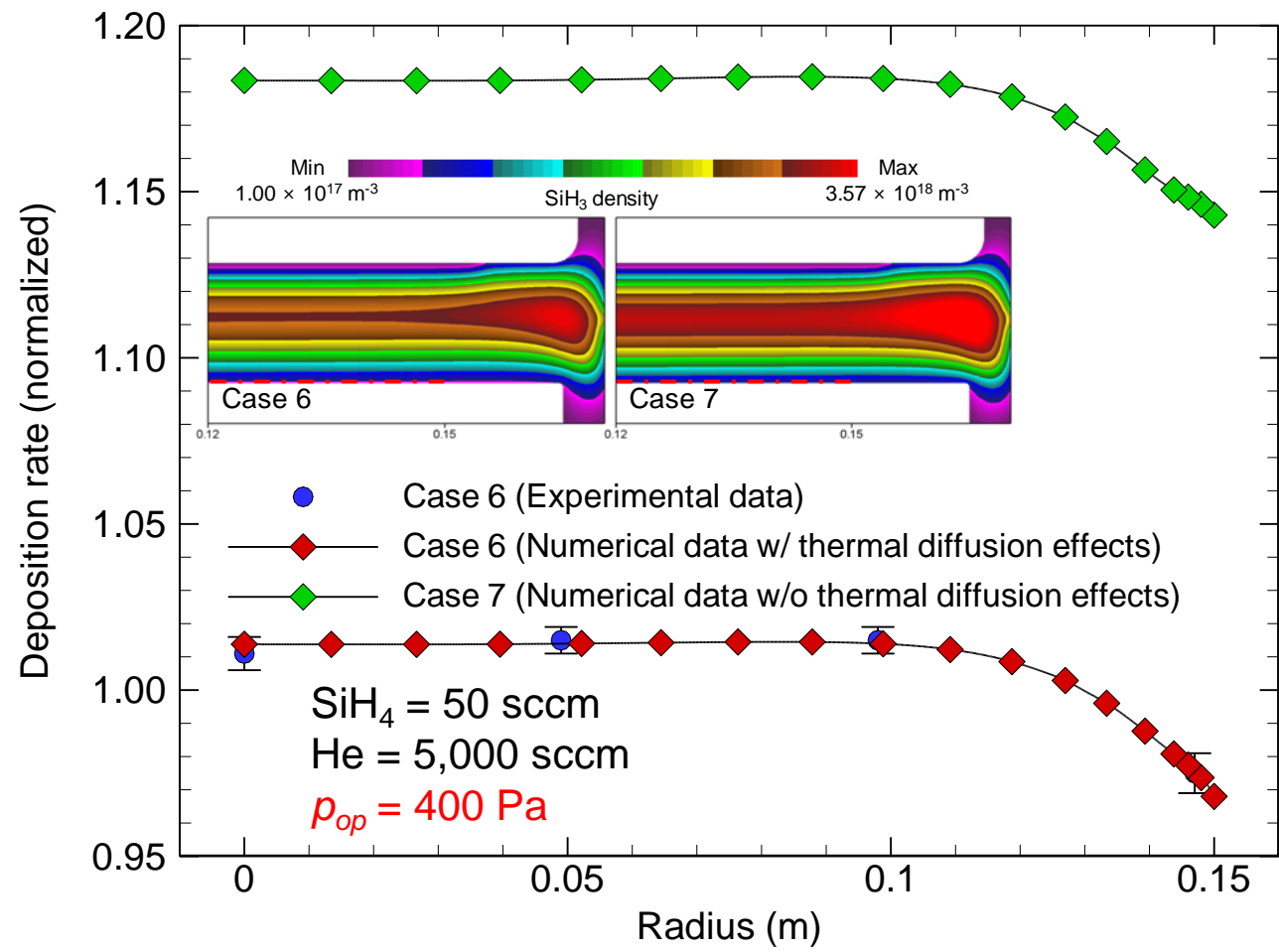
$$C_{ij}^* = \Omega_{ij}^{(1,2)*} / \Omega_{ij}^{(1,1)*}$$

$$\sigma_{ij} = (\sigma_i + \sigma_j) / 2$$



Effects of the thermal diffusion

$T_{sh} = 473\text{ K}$
 $T_{sw} = 423\text{ K}$
 $T_s = 673\text{ K}$

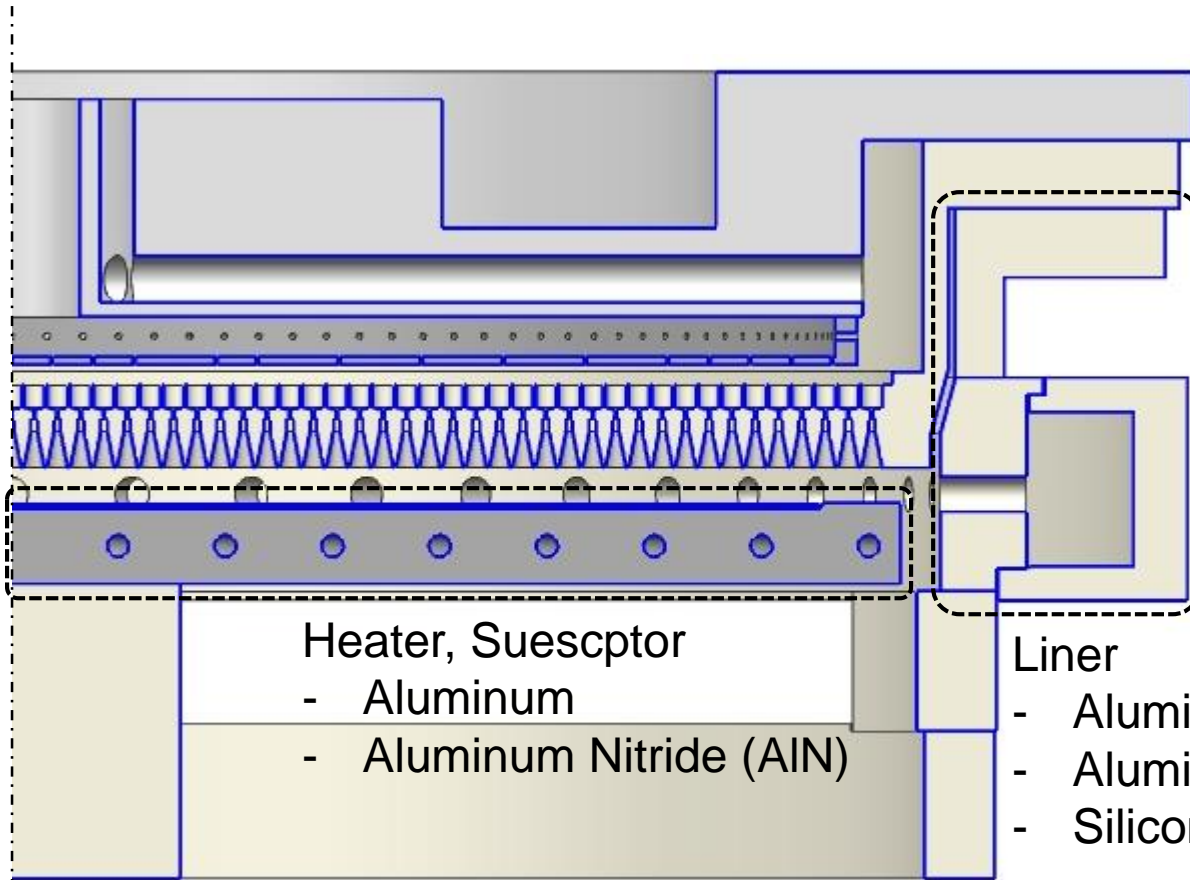


Simulated deposition rates measured along the radial direction are given for Cases 6 (red diamond) and 7 (green diamond). In addition, the experimental data for Case 6 (blue circle) are superimposed. For Case 6, the numerical and experimental data are both normalized to their corresponding averaged values. However, the profile of Case 7 is normalized to the averaged value of the profile of Case 6 to serve as a quantitative comparison of the deposition rates. A deposition rate discrepancy of about 17% can be seen between Cases 6 and 7. The inset depicts the spatial variations of SiH₃ densities for Cases 6 and 7; the SiH₃ density of Case 6 is lower than that of Case 7 near the “hot susceptor.”

These two methods can have
“the chemistry dependency.”

Then, which method can be more
“physically general?”

Sidewall and electrode spacing



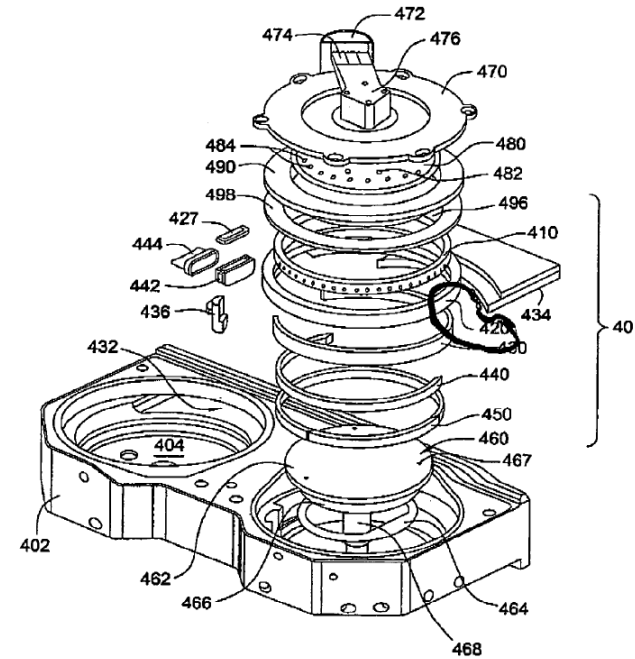
Centerline of
reactor

Heater, Susceptor

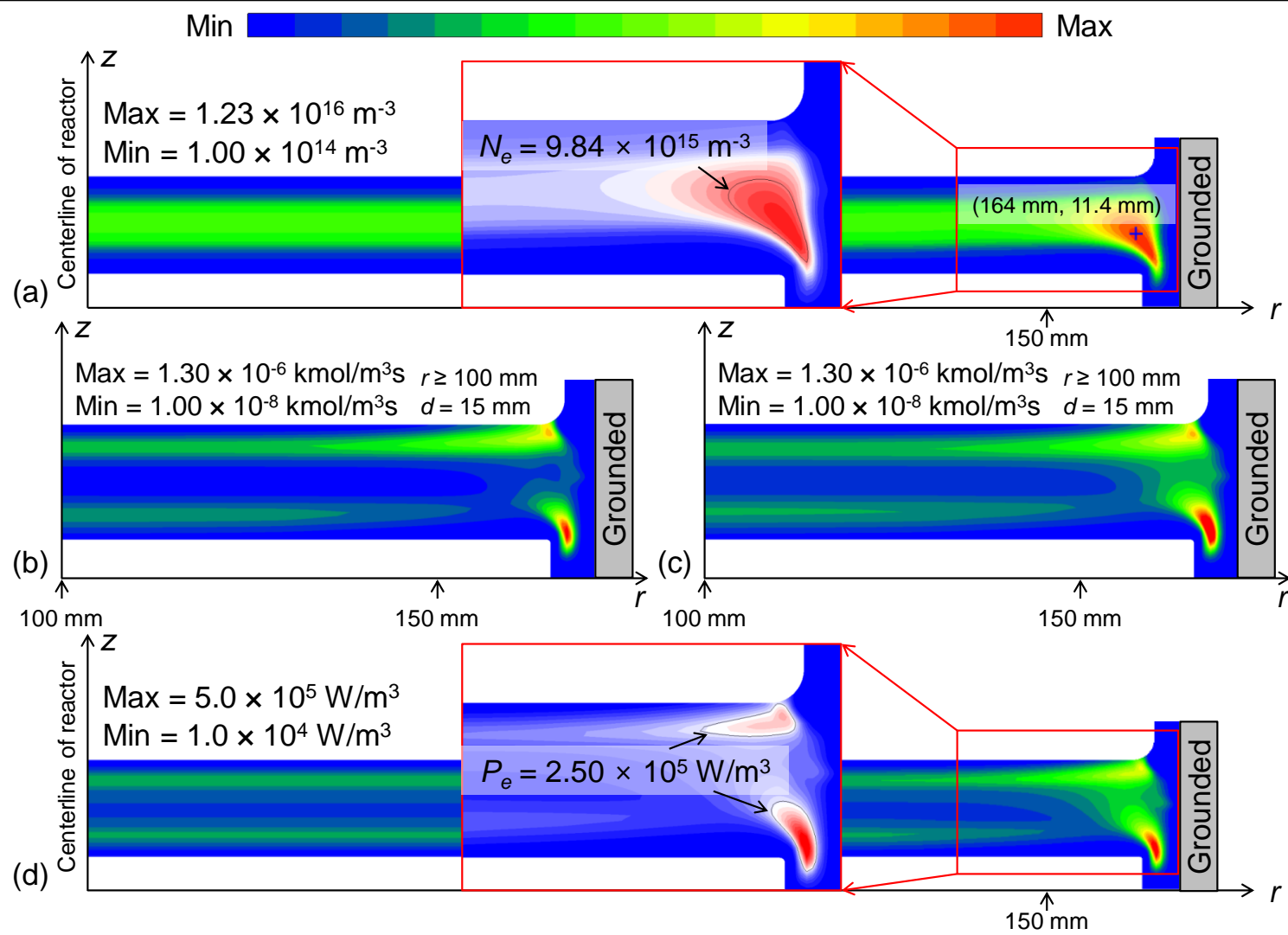
- Aluminum
- Aluminum Nitride (AlN)

Liner

- Aluminum
- Aluminum Oxide (Al₂O₃)
- Silicon Carbide (SiC)

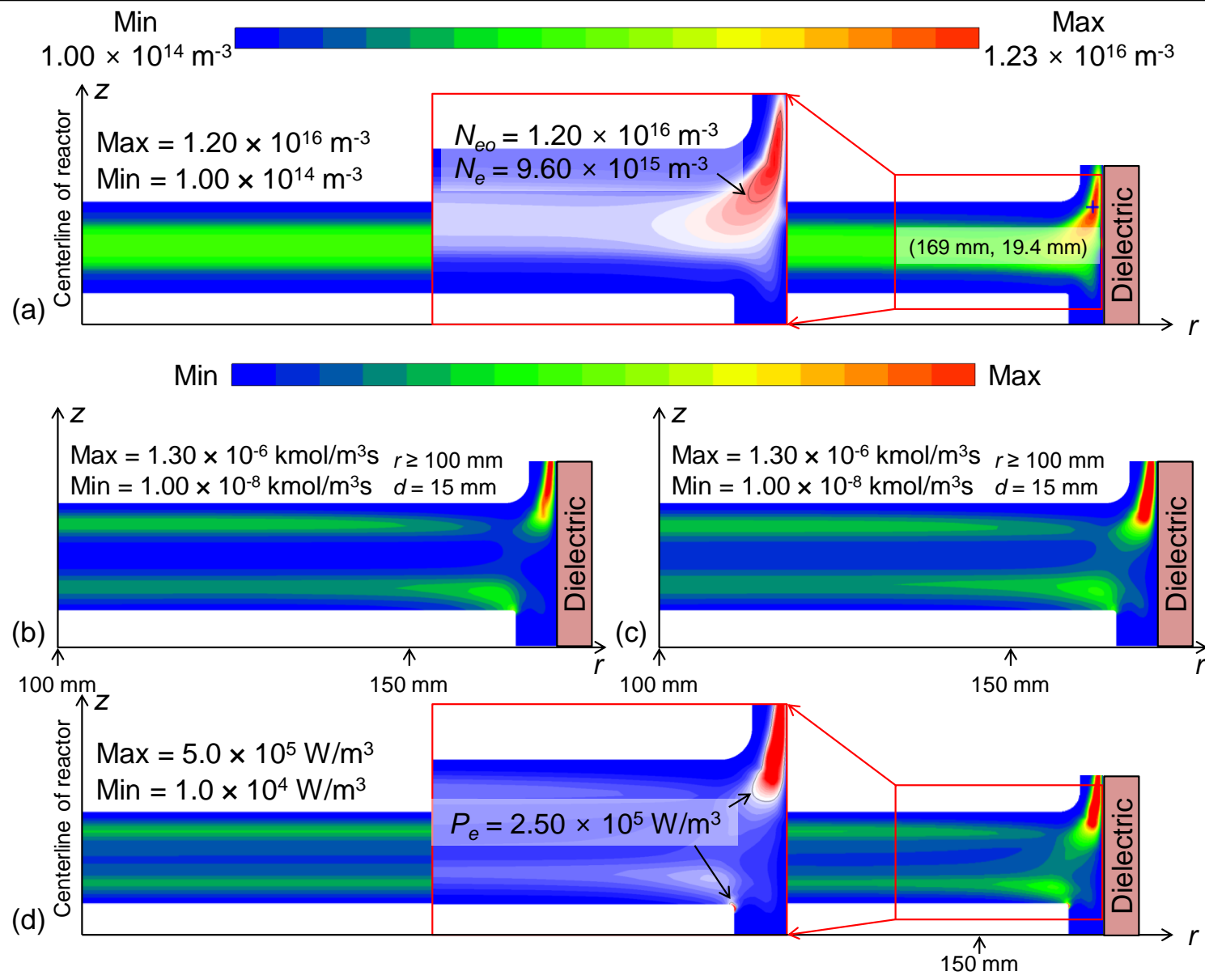


Sidewall effects: SiH₄/NH₃/N₂/He mixture

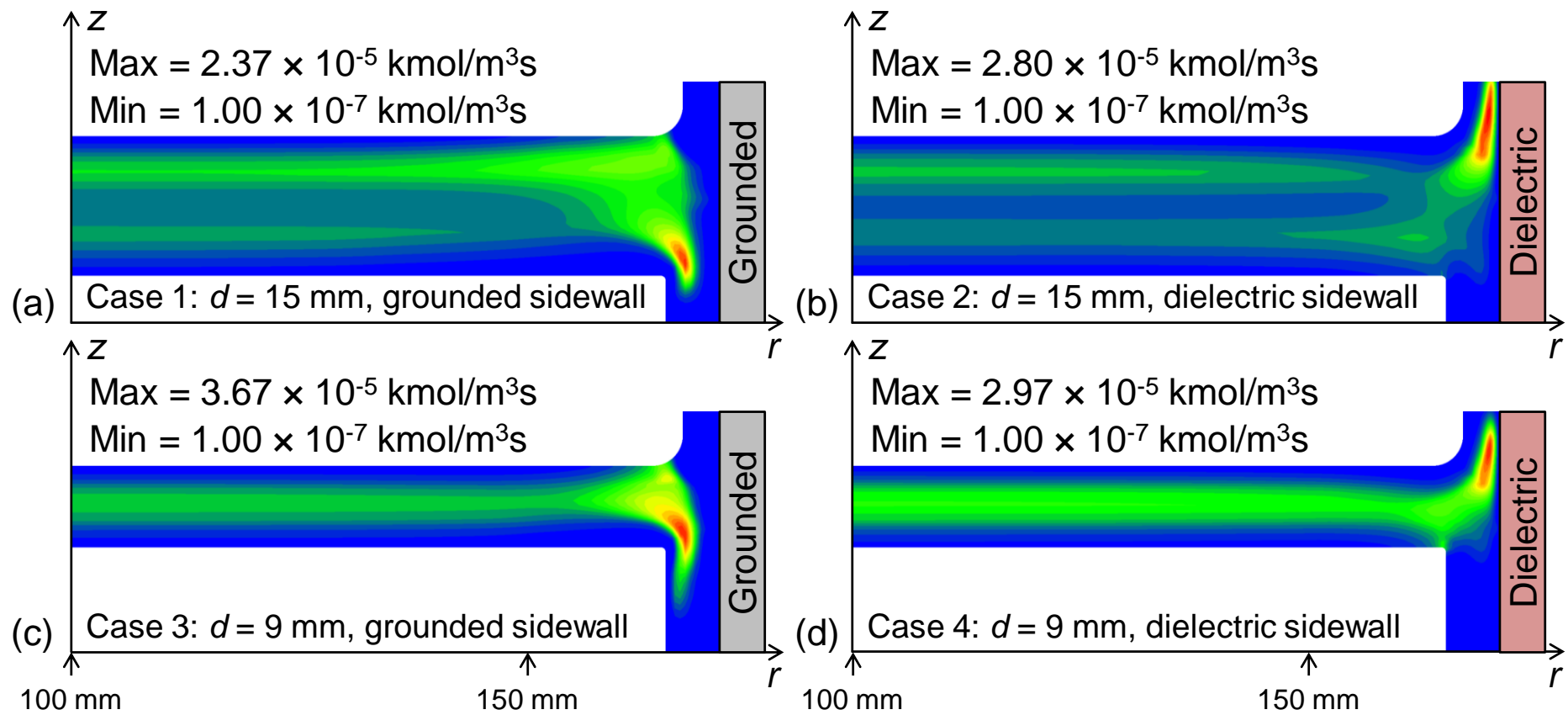


Contour plots of spatial variations in the time-averaged (a) electron density, N_e , (b) ionization rate of SiH₂⁺, (c) ionization rate of NH₃⁺, and (d) electron power density, P_e for case with the grounded sidewall. The profiles are radially uniform at $r < 100\text{mm}$ as shown in (a) and (d), and thus (b) and (c) are shown only for $r \geq 100 \text{ mm}$.

Sidewall effects: SiH₄/NH₃/N₂/He mixture

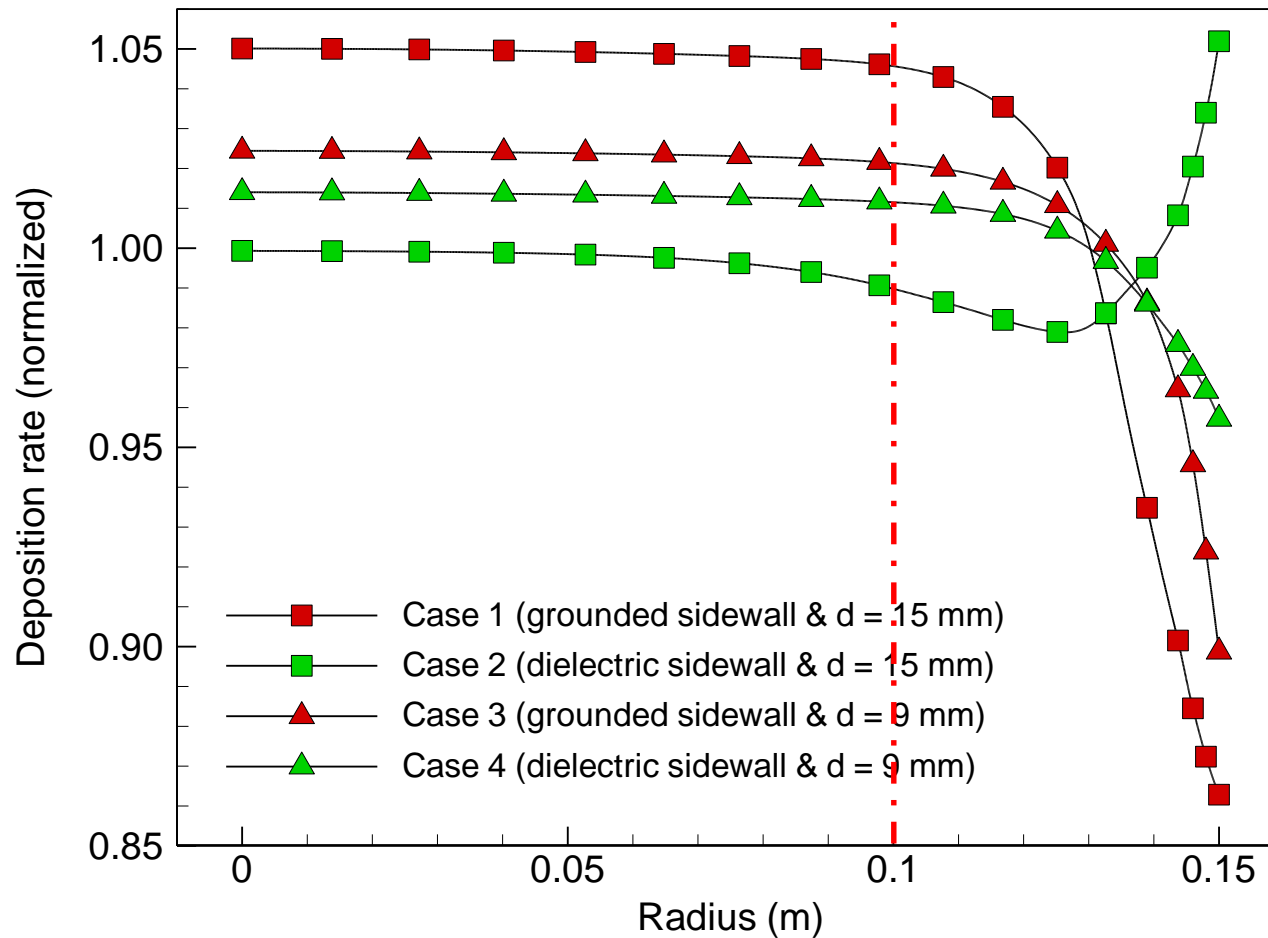


Sidewall effects: SiH₄/NH₃/N₂/He mixture



Contour plots of the time-averaged dissociation rates of SiH₄ molecules ($e^- + \text{SiH}_4 \rightarrow \text{SiH}_3 + \text{H} + e^-$) for (a) case 1, (b) case 2, (c) case 3, and (d) case 4. As the profiles are radially uniform for $r < 100$ mm, contours are shown only for $r \geq 100$ mm.

$\text{SiH}_4/\text{NH}_3/\text{N}_2/\text{He}$ mixture



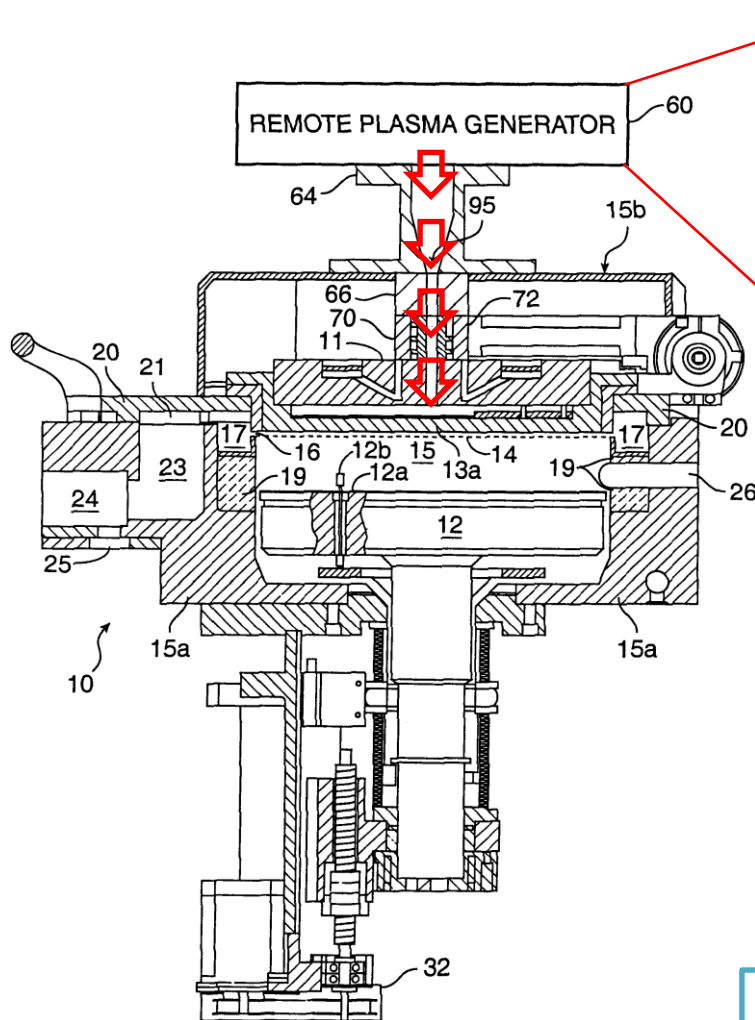
Normalized deposition rate profiles for cases 1, 2, 3, and 4. Owing to the axi-symmetry of the reactor, the simulated deposition rate profiles are plotted along the electrode radius.

Concluding remarks

- In this study, we numerically demonstrated that modulation of the sidewall conditions could contribute to controlling distributions of the plasma variables in an intermediate pressure CCP-PECVD.
- A cylindrical discharge volume was set to be radially surrounded by a lateral sidewall. To vary the sidewall conditions, we toggled its electrical condition from grounded to dielectric.
- Some important findings were observed.
 - ✓ First, we found that the case with the grounded sidewall has the spatial distributions of the ionization rate, ion and electron densities more heavily weighted toward the larger radius than the cases with the thick insulator.
 - ✓ By utilization of the thick insulator, noticeable reduction of the peak ionization rate could be achieved near the sidewall without significant changes of the ion and electron densities in the inter-electrode region.
 - ✓ These observations were owing to the fact that the effective size of the electrode of the case with the thick insulator becomes more comparable due to the higher impedance of the sidewall, as compared with that of the case with the grounded sidewall.
 - ✓ As a result, the thick insulator induced significant improvement in the uniformity of the deposition rate profile.

Other Works

Remote plasma cleaning (RPC)



Reaction pathways	Description
$e + \text{NF}_3 \rightarrow e + \text{NF}_2 + \text{F}$	Direct electron impact dissociation
$e + \text{NF}_3 \rightarrow \text{NF}_2 + \text{F}^-$	Electron impact dissociative attachment
Excitation and successive dissociation	
$e + \text{NF}_3 \rightarrow e + \text{NF}_3^a + e$	Vibrational and electronic excitation
$e + \text{NF}_3^a \rightarrow \text{NF}_2 + \text{F}$	Dissociative attachment after excitation
$e + \text{NF}_3^a \rightarrow +\text{NF}_2 + \text{F} + e$	Dissociation from excitation
Thermal pathway	
$\text{NF}_3 + \text{M} \rightarrow \text{NF}_2 + \text{F} + \text{M}$	Thermal dissociation

^a Indicates an electronically or vibrationally excited state.

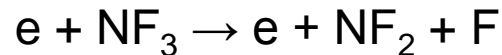
- Remote NF_3 plasmas have now been adopted for cleaning most CVD/ALD reactors due to faster clean times, reduced reactor damage and substantially lower emissions of gases having high GWPs.
- An NF_3 plasma is generated upstream of the reactor, generating F atoms that are then transported to the reactor where they react with the residue such as SiO_x or SiN_x covering the reactor surfaces.
- Since the discharge is confined to the plasma source, the surfaces of the chamber are not exposed to a flux of energetic ions.
- Hence, the residues are cleaned by a chemical etch.

Number densities of reactive radicals are calculated in the RPG model and their flux values are introduced as a boundary condition of reactor inlet.

Reference:
Integration of remote plasma generator with semiconductor processing chamber
US 6387207 B1

► Plasma Chemistry

NF₃ Dissociation: $e + \text{NF}_3 + \text{Ar} \rightarrow e + \text{NF}_2 + \text{F} + \text{Ar} + \text{Ar}^* + \dots$



► Radical Chemistry

1. Gas Phase Reaction

Volume Recombination: $\text{F} + \text{F} + \text{M} \rightarrow \text{F}_2 + \text{M}$

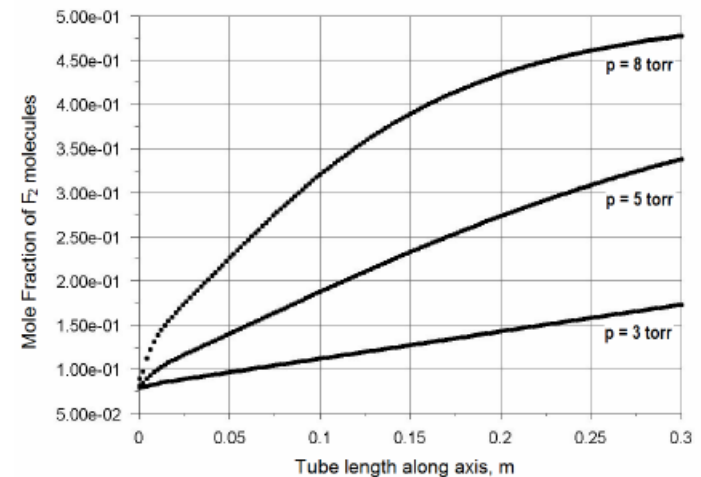
2. Surface Reaction

Surface Adsorption: $\text{F} \rightarrow \text{F}_s$

Surface Recombination: $\text{F} + \text{F}_s \rightarrow \text{F}_2$

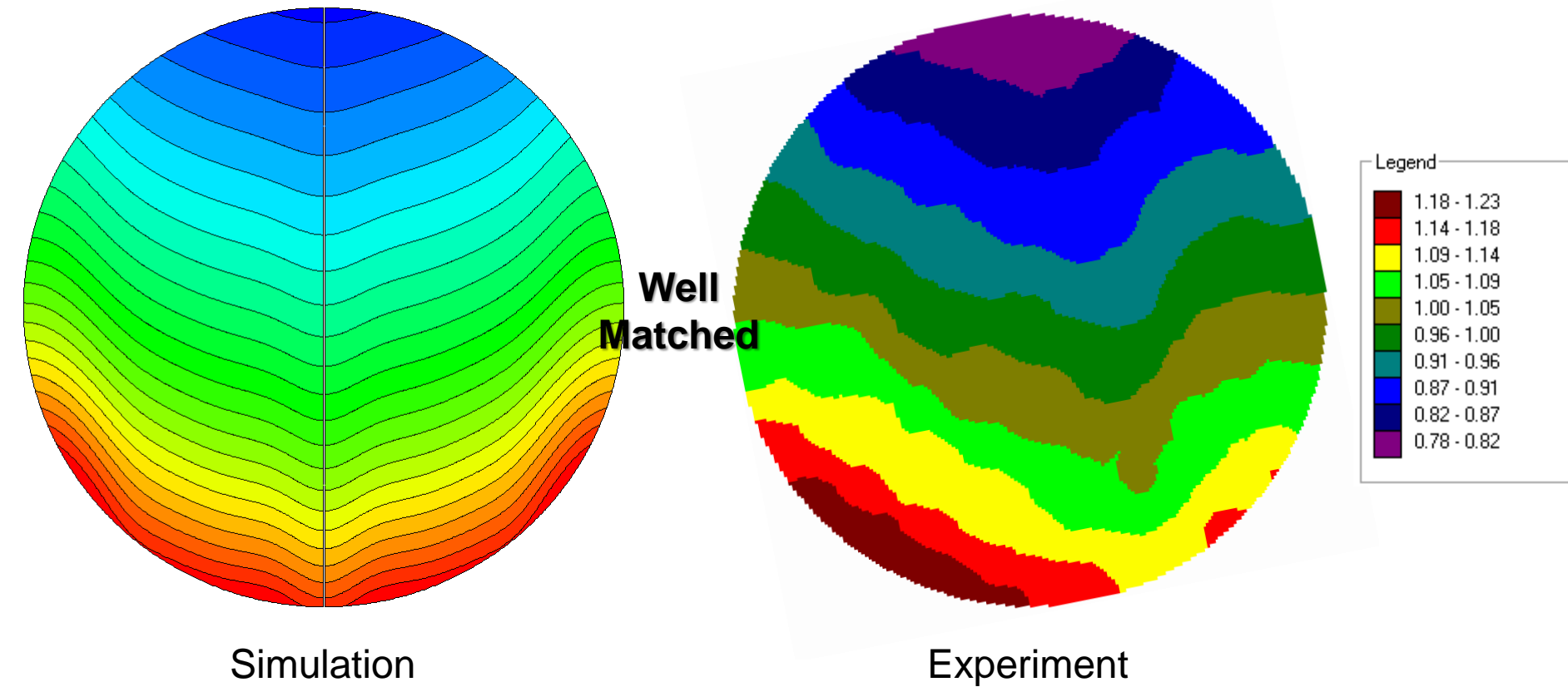
Surface Desorption: $\text{F}_s \rightarrow \text{F}$

Oxide Etching: $\text{SiO}_2 + 4\text{F} \rightarrow \text{SiF}_4 + \text{O}_2$



Mole fractions of F₂ molecules in transport tube length. The curves show computed values for three different pressures: 3, 5 and 8 Torr.

Remote plasma cleaning (RPC)



Thank you