SCALING OF LOW-PRESSURE IONIZED METAL PVD REACTORS*

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AGENDA

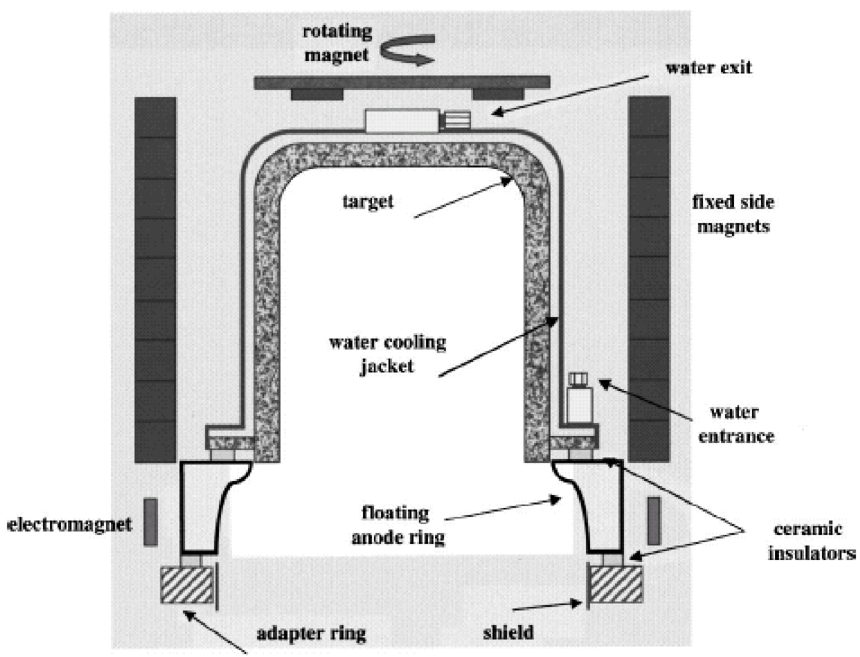
- Simulation of Ionized Metal PVD (IMPVD) Reactors
- Ion/Neutral Monte Carlo Simulation
- Scaling of IMPVD Reactors
    - Pressure
    - Magnetic Field Configuration
    - Magnetic Field Strength
    - Power
    - Cu seed layer deposition
- Concluding remarks

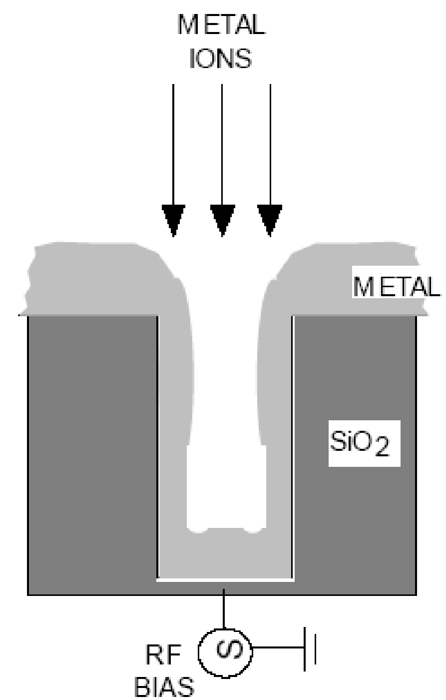
IONIZED METAL PHYSICAL VAPOR DEPOSITION

- **IMPVD is increasingly being used to deposit diffusion barriers and seed layers onto high aspect ratio trenches.**

- **As IMPVD operates over a range of pressures (< 1 mTorr to 40 mTorr), analysis requires wide range of capabilities.**

HOLLOW CATHODE MAGNETRON SOURCE*





*Klawuhn et al., J. Vac. Sci. Technol. A 18 (4), 1546 (2000)

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CHALLENGES OF SIMULATING IMPVD

- At HCM pressures (< 1 mTorr – 10's mTorr), conventional continuum simulations are questionable as transport is highly non-equilibrium.
  - Kn = $\lambda/L \approx 1$ at 1 mTorr

- Simulation of Plasmas:
  - Low Pressure: Kinetic (i.e. Solve Boltzmann's Equations)
  - High Pressure: Continuum Equations

- In principle, continuum equations are simply moments of the Boltzmann's equation. If the distribution functions are known, the equations should be valid at low pressures.

- A hybrid modeling approach has been developed in which the ion and neutral temperatures are kinetically derived and implemented in fluid equations.

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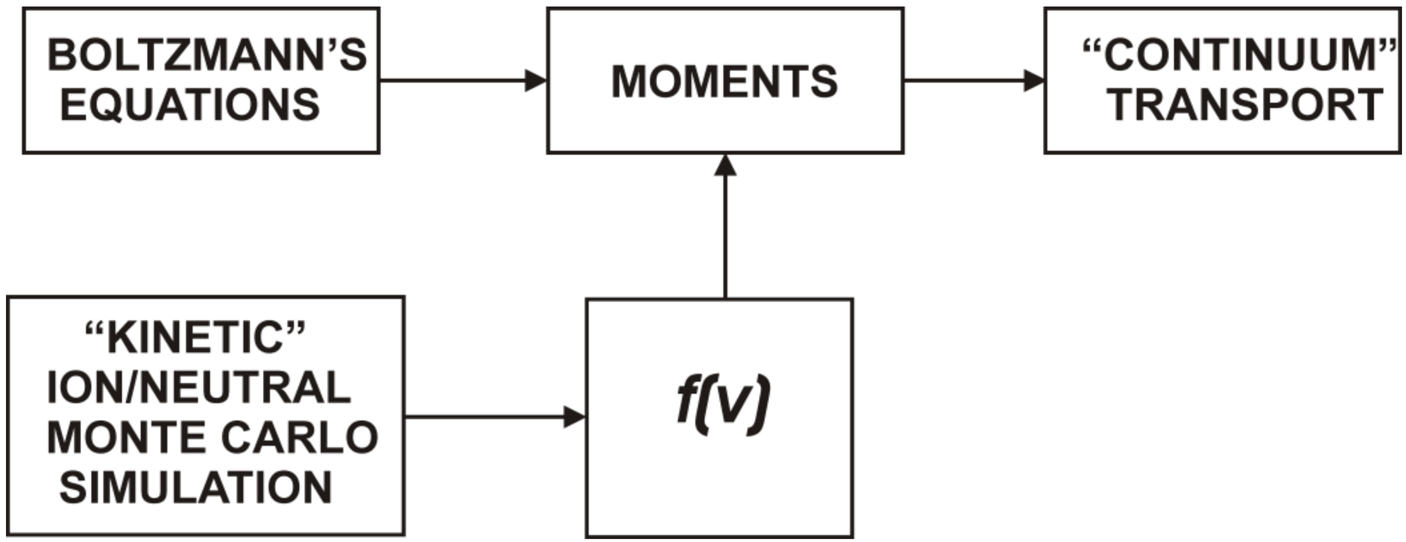
DESCRIPTION OF HYBRID METHOD



- **An ion/neutral Monte Carlo simulation is used to compute the transport coefficients for computing moments of the Boltzmann's equation.**

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HYBRID PLASMA EQUIPMENT MODEL (HPEM)

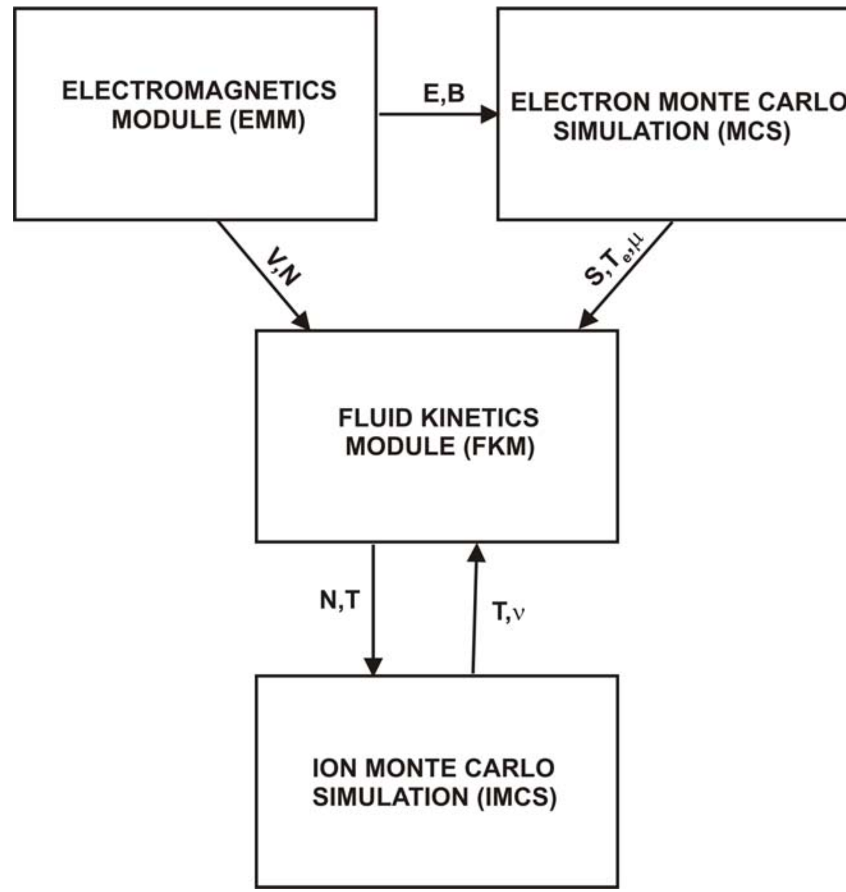
- HPEM is a modular simulator of low pressure plasmas.

- EMM: inductively coupled electric and magnetic fields.

- MCS: EEDs, transport coefficients and source functions.

- FKS:
  Ions: Continuity, Momentum
  Neutrals: Continuity,Momentum
  Electrons: Drift Diffusion, Energy
  Electric Potentials: Poisson’s Equation

- IMCS: ion/neutrals transport coefficients.



HYBRID PLASMA EQUIPMENT MODEL (HPEM)

- **Continuity (heavy species) :**

$$\frac{\partial N_i}{\partial t} = \nabla \cdot \left(N_i \vec{v}_i\right) + S_i$$

- **Momentum (heavy species) :**

IMCS

$$\frac{\partial \left(N_i \vec{v}_i\right)}{\partial t} = \frac{q_i}{m_i} N_i \left(\vec{E}_s + \vec{v}_i \times \vec{B}_s\right) - \frac{1}{m_i} \nabla P_i + \sum_j N_i N_j k_{ij} \left(\vec{v}_j - \vec{v}_i\right) - \nabla \cdot \bar{\bar{\tau}}_i - \nabla \cdot \left(N_i \vec{v}_i \vec{v}_i\right)$$

- **Energy (heavy species) :**

IMCS

OR

$$\frac{\partial N_i c_v T_i}{\partial t} = \nabla \cdot \kappa_i \nabla T_i - P_i \nabla \cdot \vec{v}_i - \nabla \cdot (\vec{\varphi}_i \varepsilon_i) + \frac{N_i q_i^2}{m_i \nu_i} E_s^2 + \frac{N_i q_i^2 \nu_i}{m_i (\nu_i^2 + \omega^2)} E^2 + \sum_j 3 \frac{m_{ij}}{m_i + m_j} N_i N_j R_{ij} k (T_j - T_i)$$

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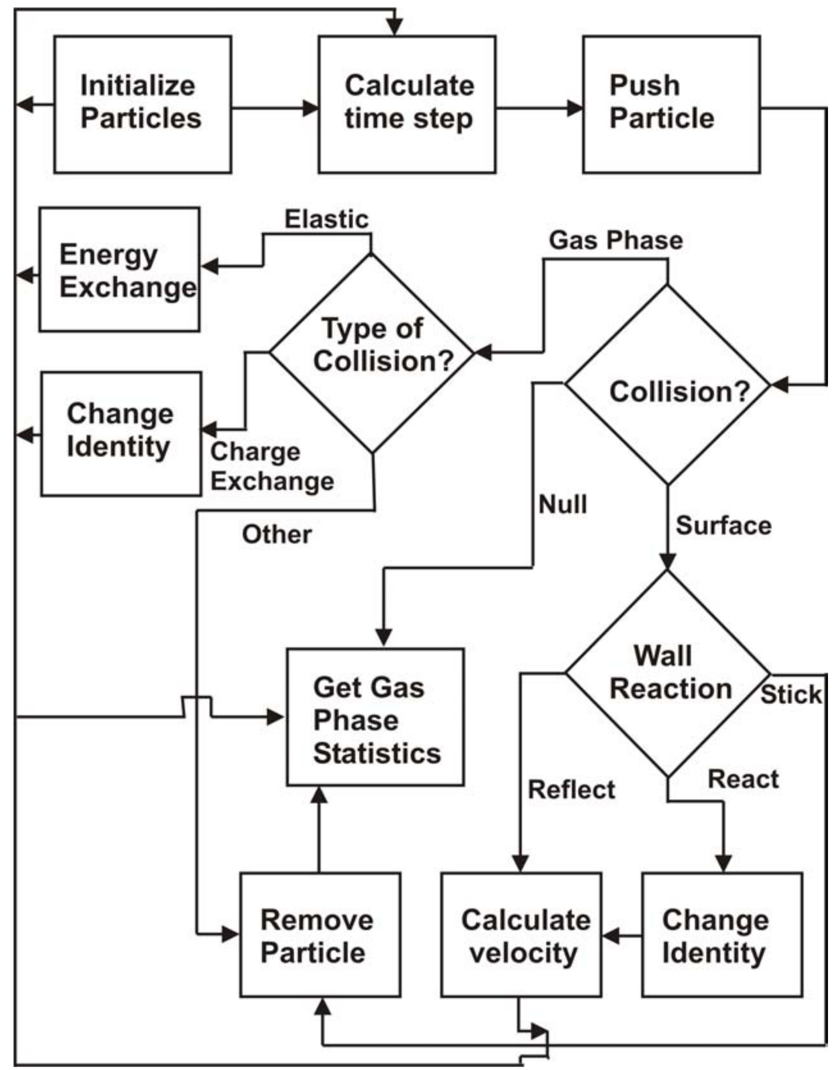
ION/NEUTRAL MONTE CARLO SIMULATION (IMCS)

- **Pseudoparticles are launched based on source functions.**
- **Particles representing the injected gas species are launched from inlet nozzles based on flow rates.**
- **Particle trajectories are followed till they reach the pump port or get consumed in a collision.**
- **Ions and neutrals striking the wall are reflected back as neutrals with a specified sticking probability.**



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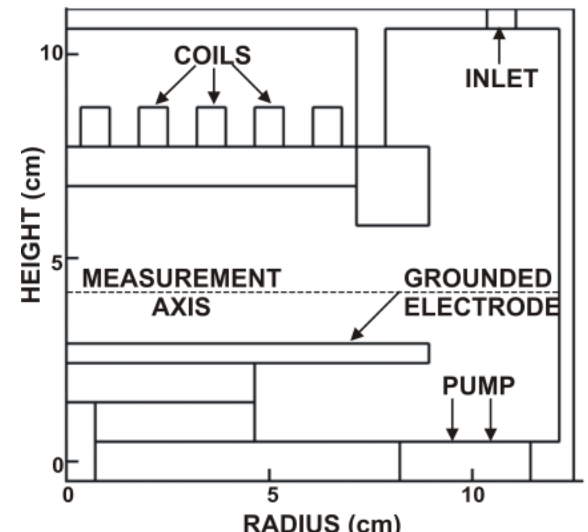
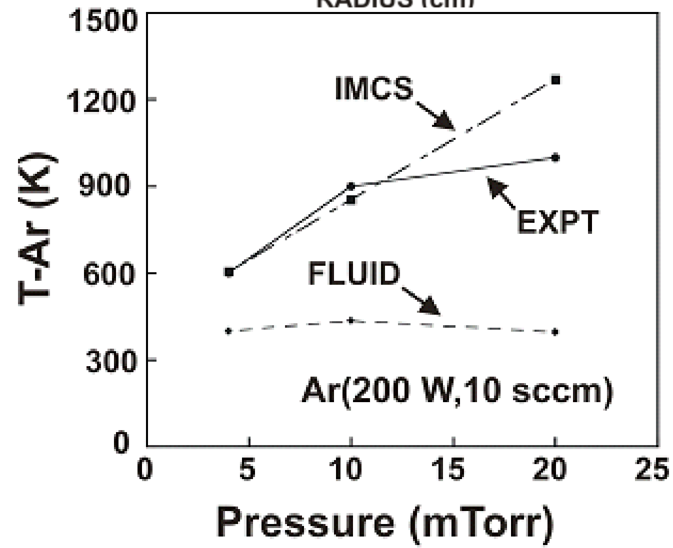
MODEL VALIDATION : GAS TEMPERATURE

- The model was validated by comparison of gas temperatures in a GEC Reference cell reactor*

- The dominant heating mechanism for Ar is symmetric charge exchange with energetic Ar^+ ions.

- T-Ar increases with pressure due to a higher charge exchange reaction rate.

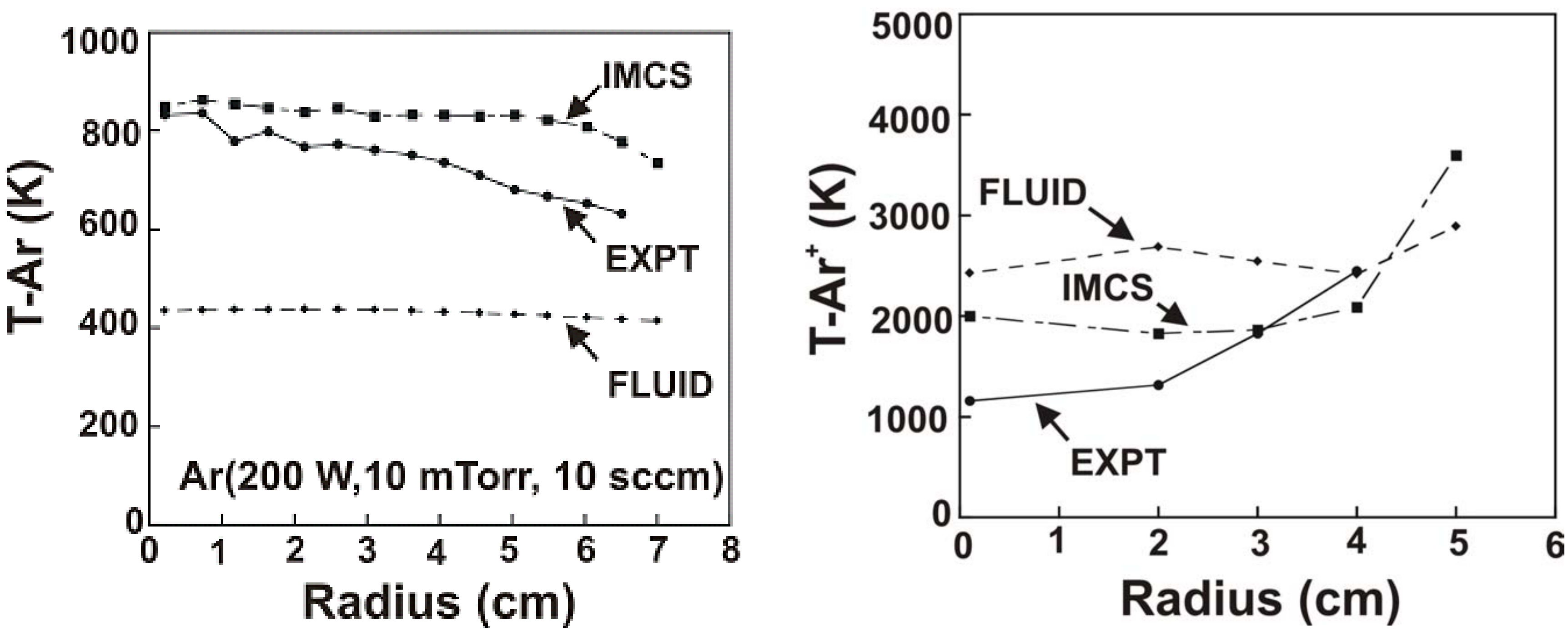




*G. A. Hebner, J. Appl. Phys. 80 (5), 2624 (1996)

MODEL VALIDATION : ION TEMPERATURE

- T-Ar peaks in the center of the reactor due to higher Ar^+ density.
- T-Ar^+ increases with radius due to the larger electric fields at the periphery of the reactor.



Ar (200 W, 10 mTorr, 10 sccm)

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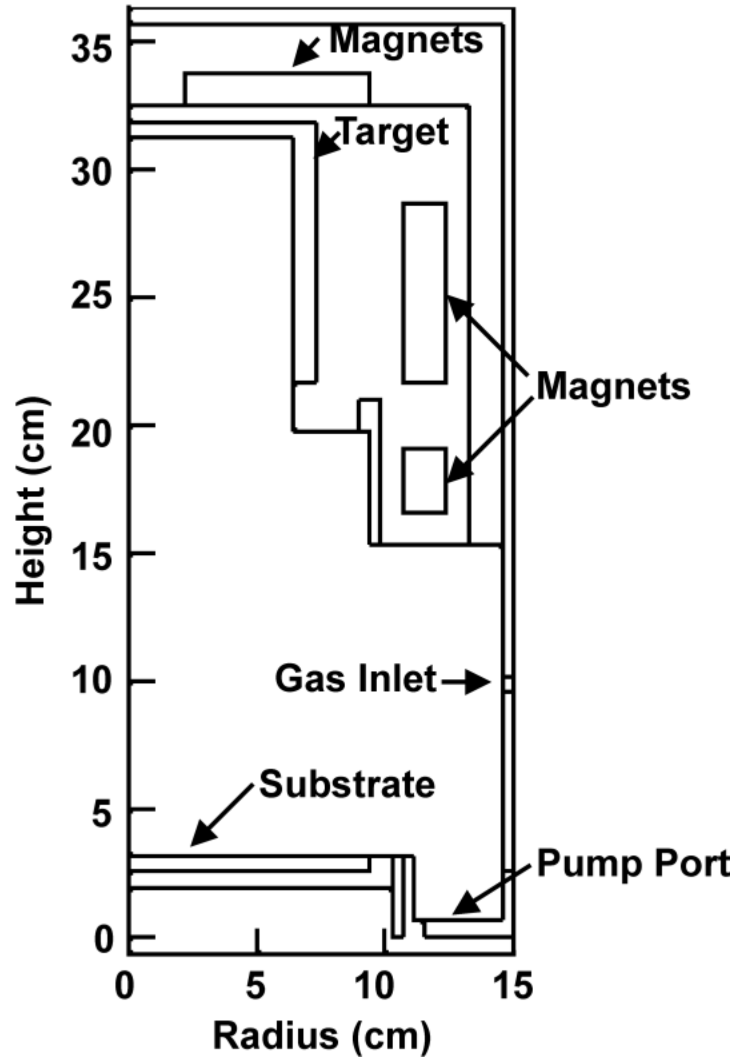
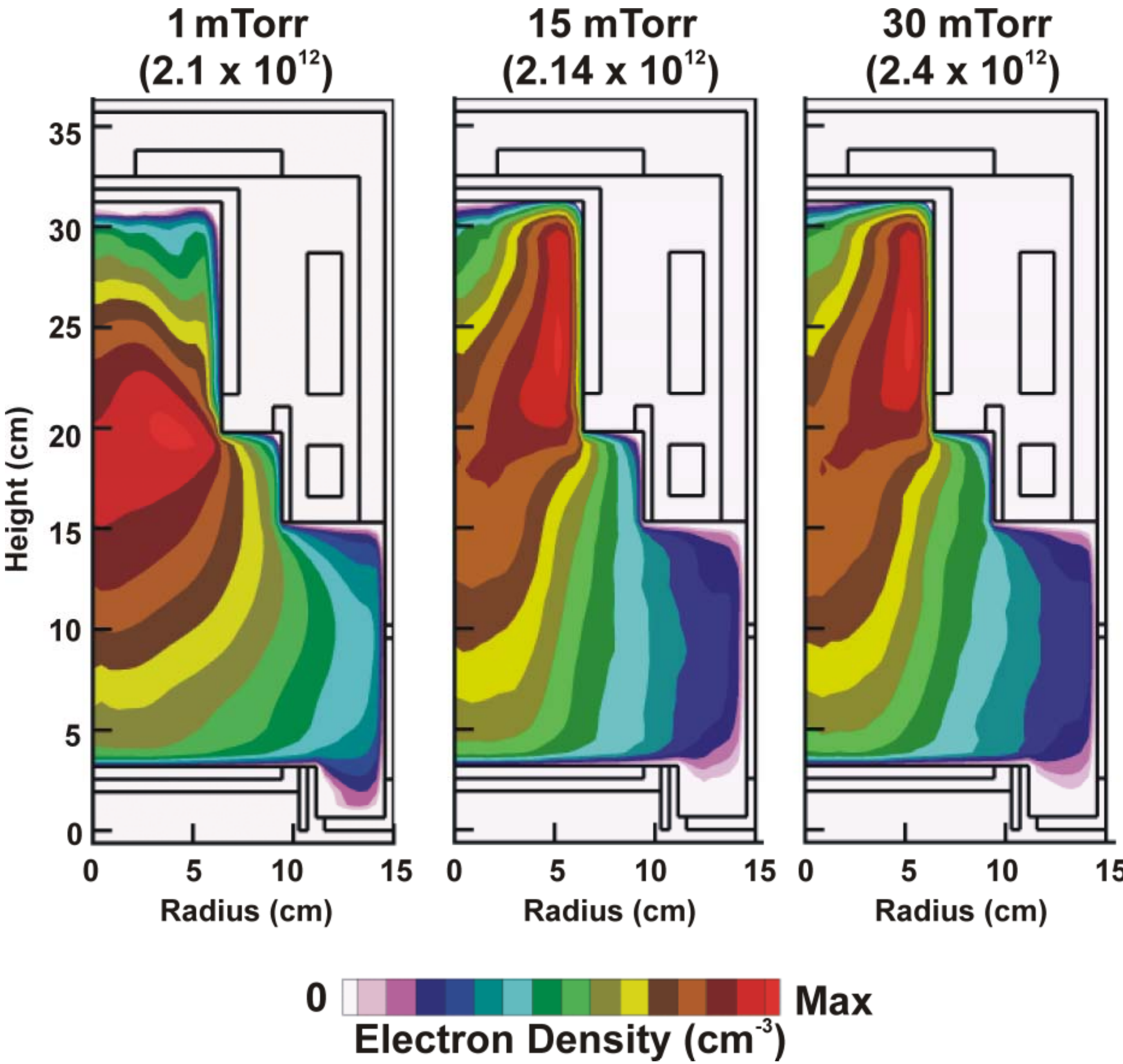
OPERATING CONDITIONS

- **Pressures: 1 – 30 mTorr**
- **Powers: 10 – 80 kW**
- **DC Bias: 150 – 500 V**
- **Ar Flows: 25-250 sccm**
- **IMCS Species: Ar, Ar^+, Cu, Cu^+, Cu^***



PLASMA DENSITY: PRESSURE



- Peak in electron density decreases and shifts from the target to the center of the reactor with decrease in pressure.
- Mean free path and conductivity of electrons increase with decrease in pressure.

- 10 kW POWER

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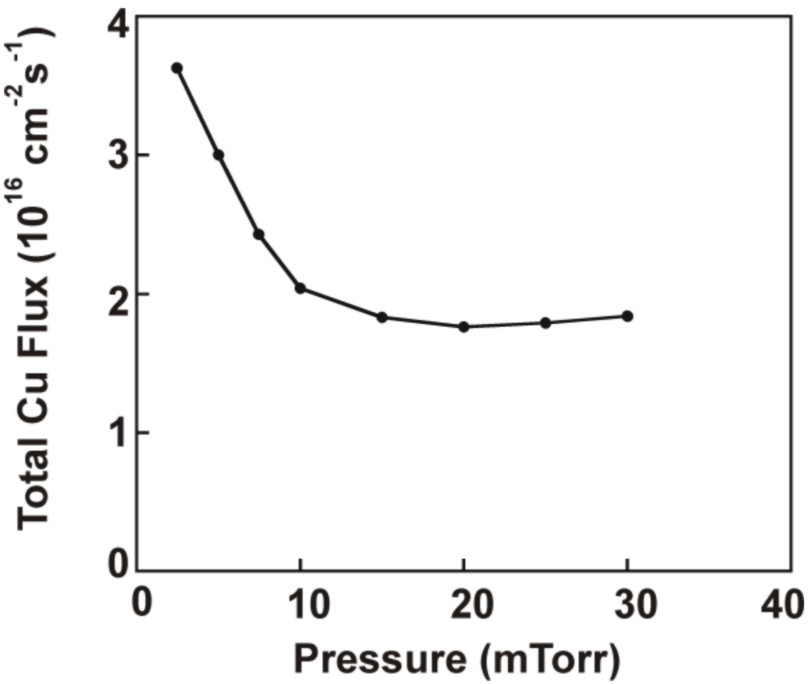
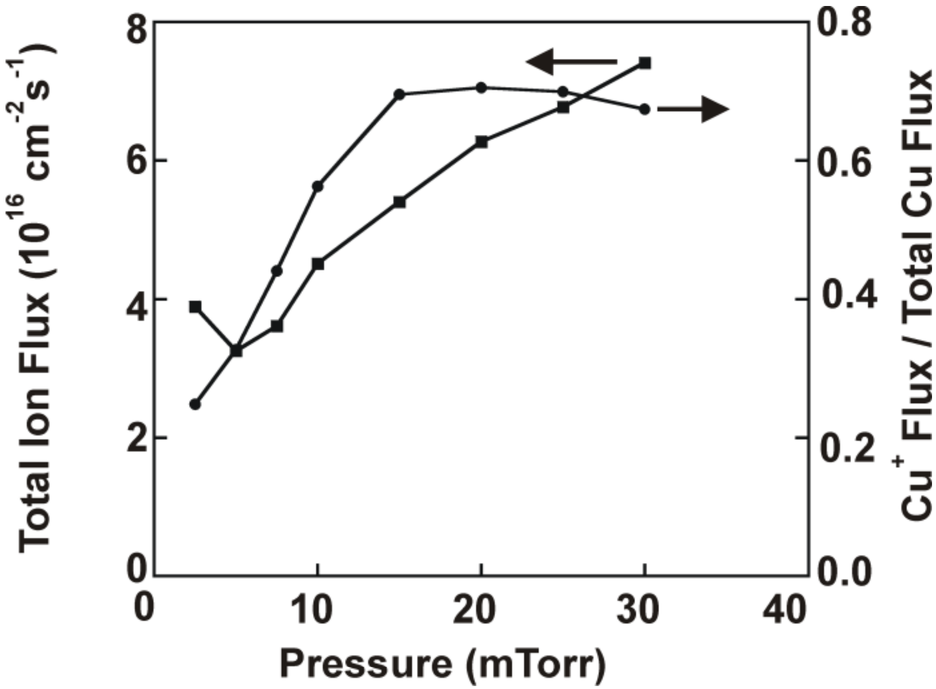
FLUXES TO SUBSTRATE : PRESSURE

- Cu flux on the wafer increases with decrease in pressure due to the larger contribution of non-thermal Cu.

- The ionized fraction of Cu flux and the total ion flux on the wafer increases with pressure due to more ionizing collisions.





- 10 kW POWER

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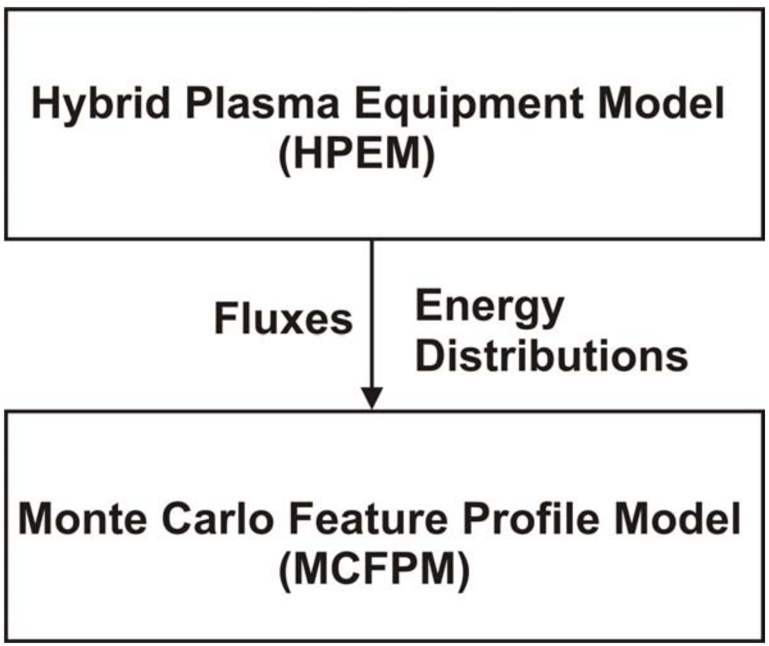
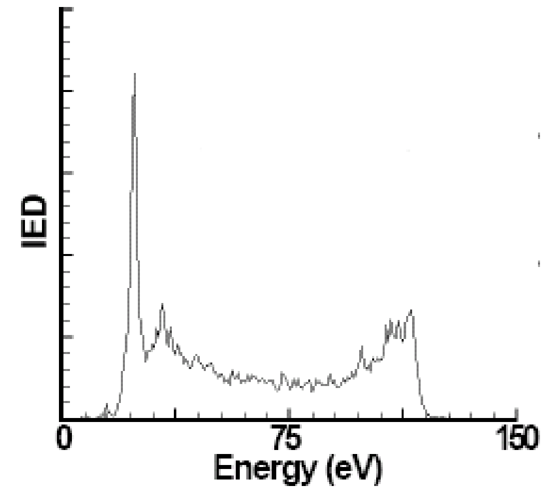
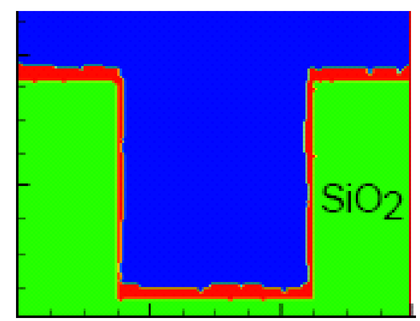
MONTE CARLO FEATURE PROFILE MODEL(MCFPM)

- **Plasma surface interactions were investigated using MCFPM.**

- **MCFPM predicts time and spatially dependent deposition profiles using ion and neutral fluxes from HPEM.**



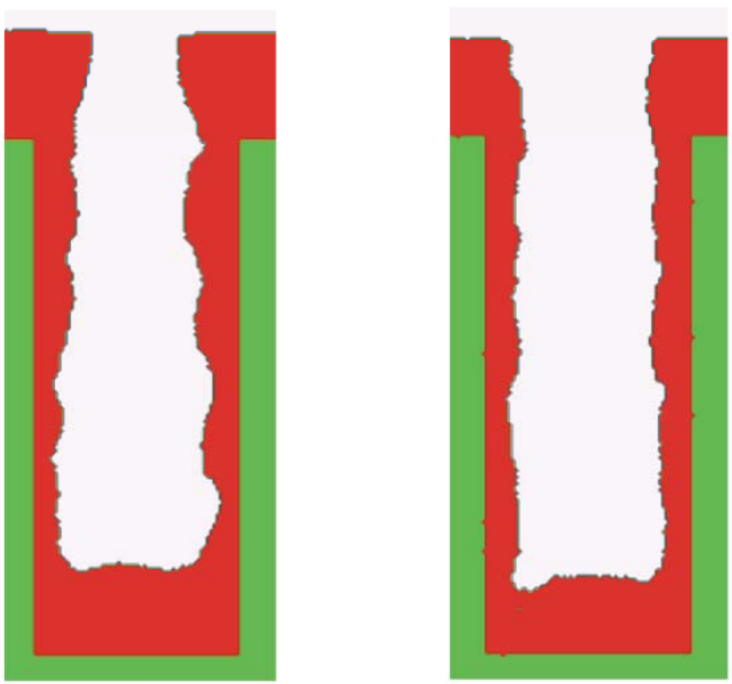




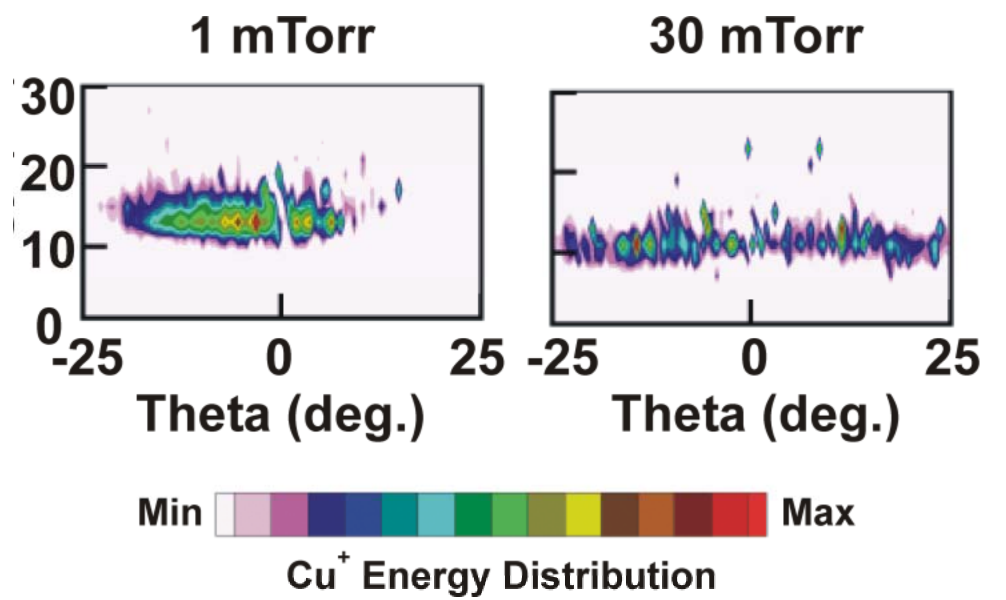
FEATURE PROFILES: PRESSURE

- Ion energies increase and IEDs narrow at lower pressures due to the increase in floating potential.
- Reduced Overhang (Side Coverage/Top Coverage) is observed at higher pressures due to higher ionization levels.

1 mTorr 30 mTorr

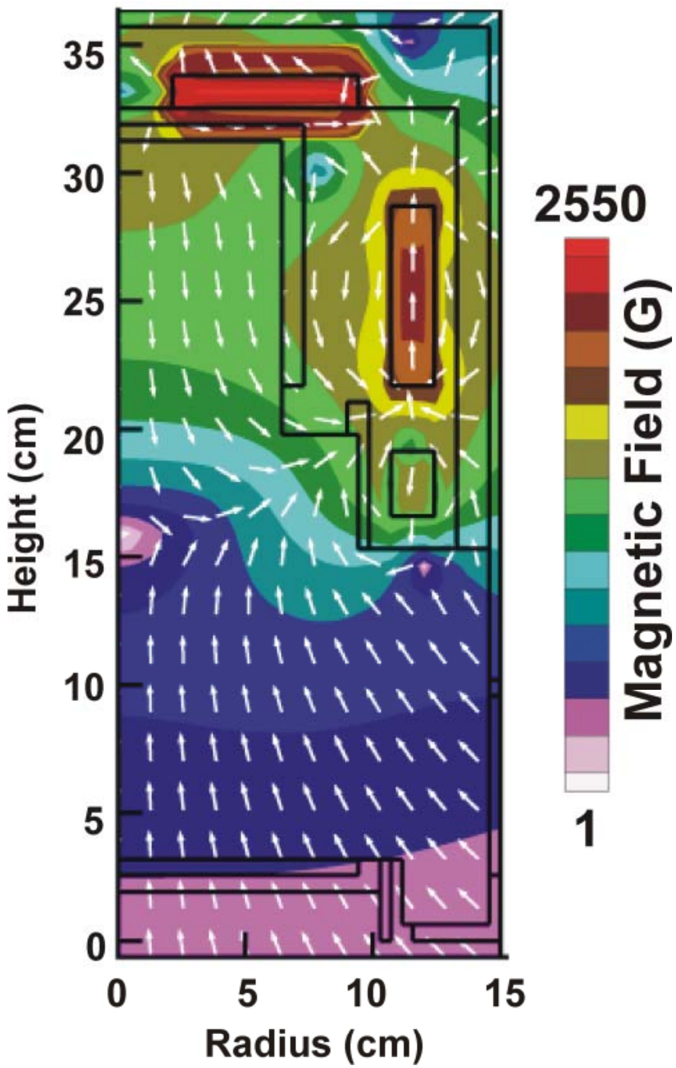


Overhang: 0.55 Overhang: 0.4



CD=65 nm, A.R. = 2.5:1

HCM : B-FIELD CONFIGURATION



- HCM relies on magnetic fields to generate high-density plasma within the volume of the cathode.
- A strong E×B force along the target surface results in efficient sputtering.
- The cusp in magnetic field near the target opening acts as an "aperture" to extract plasma from within the target volume.

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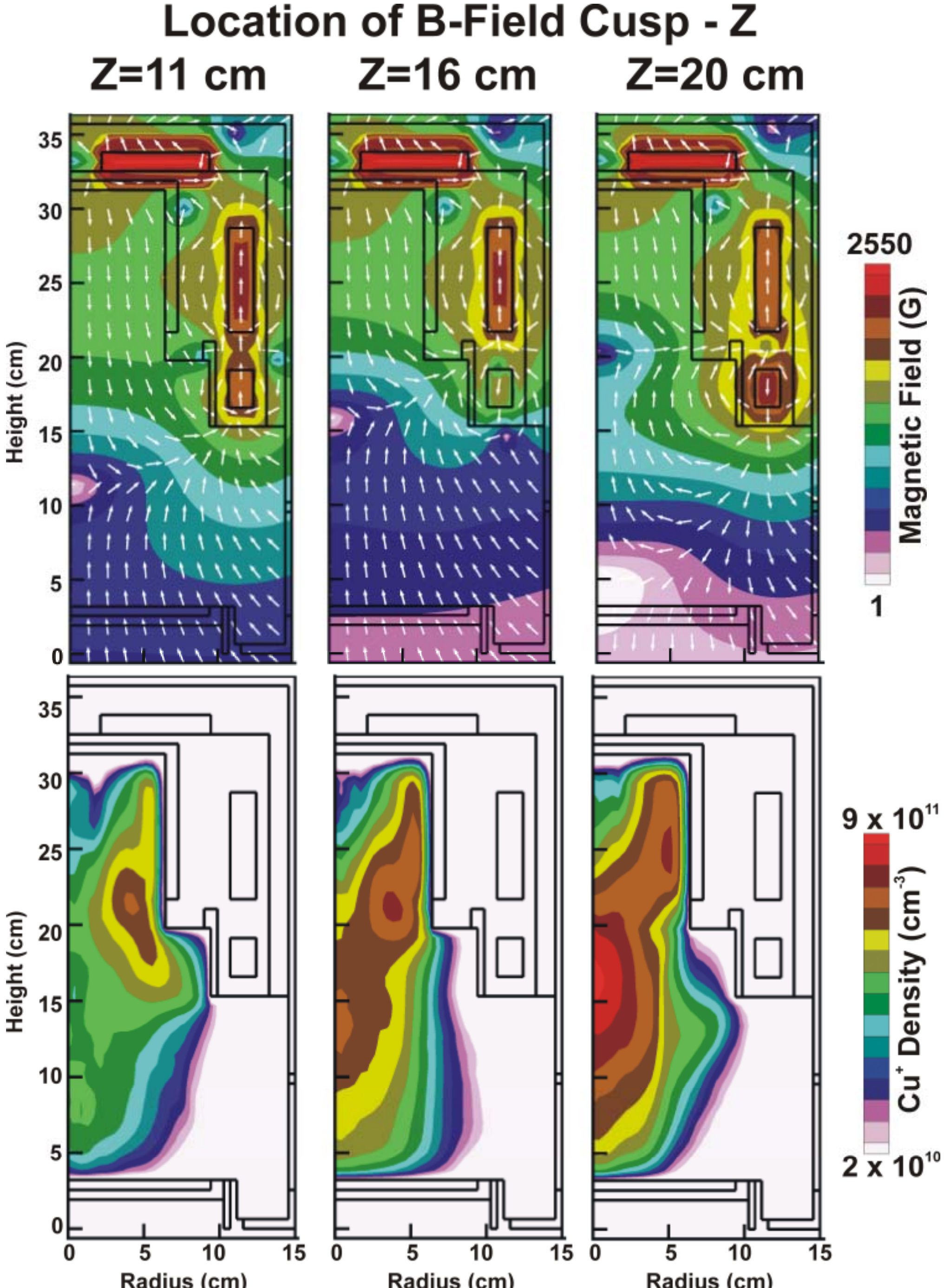

IONIZATION: B-FIELD CONFIGURATION

- As the location of cusp is moved closer to the target opening, the ionization peak increases and shifts from the target to the center of the reactor.

- 10 mTorr, 10 kW

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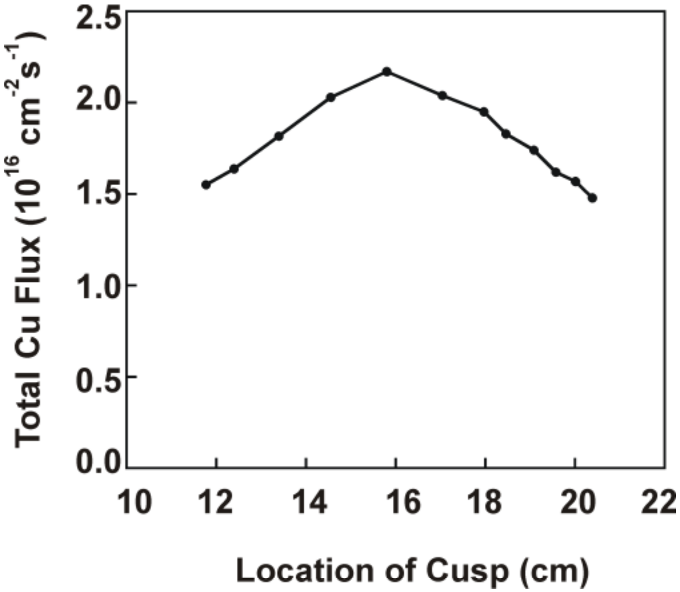
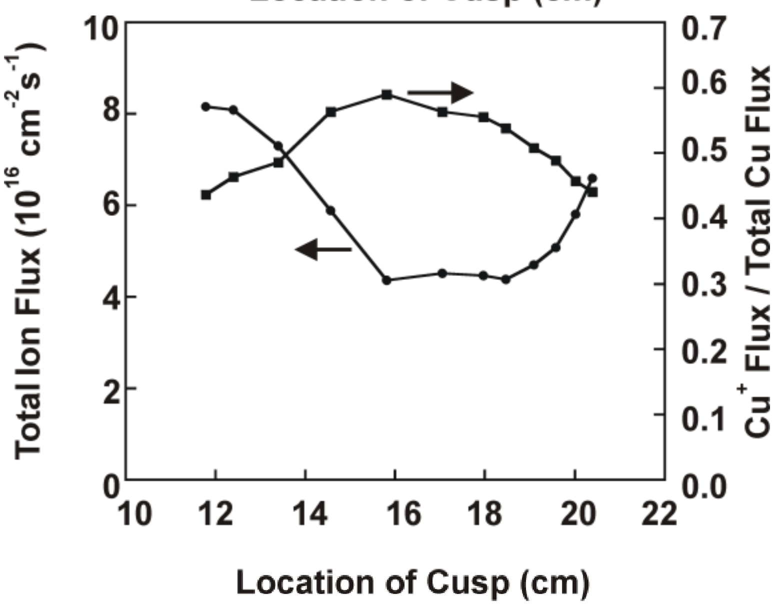
FLUXES: B-FIELD CONFIGURATION





- As the location of cusp is moved closer to the target opening, the Cu flux and Cu ion fraction increase, and the total ion flux decreases.
- At higher cusp locations, reduced magnetic confinement results is less efficient sputtering and a reduced Cu ion fraction and a larger total ion flux.

- 10 mTorr, 10 kW

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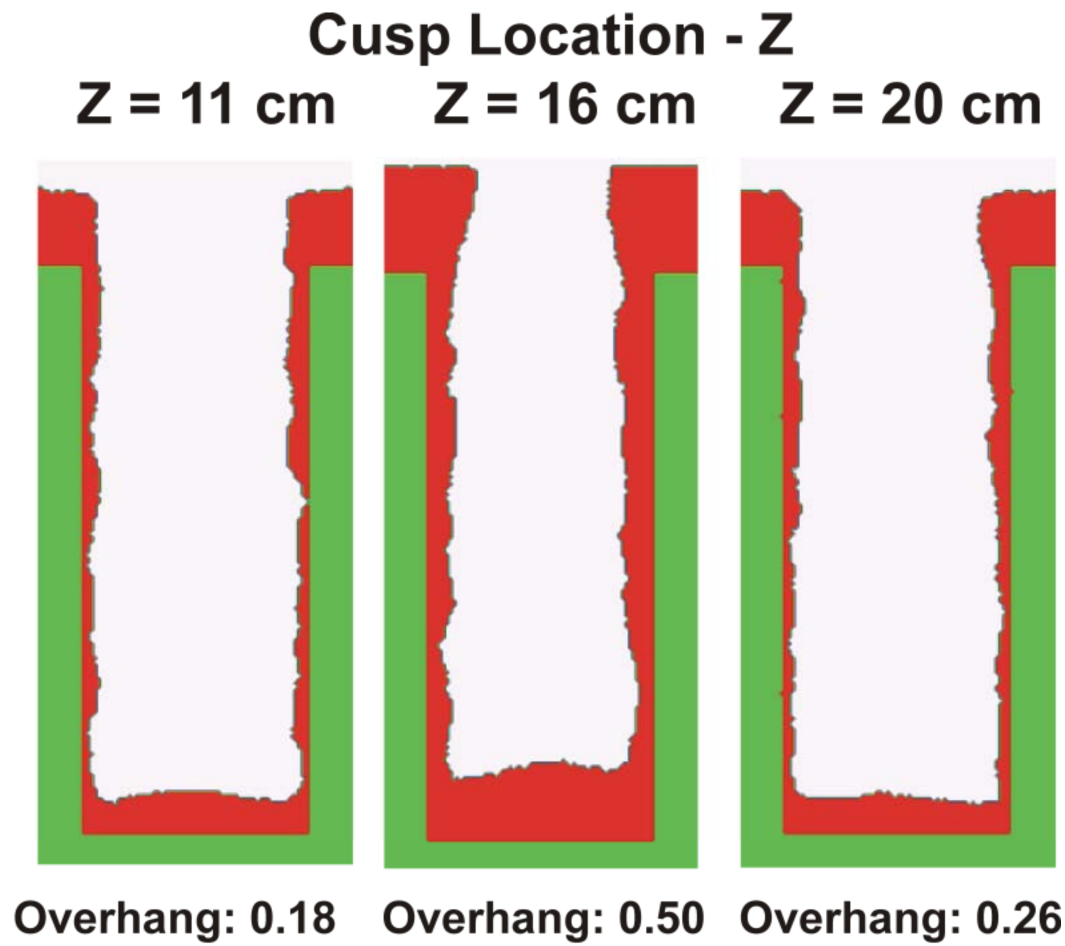
TRENCH EVOLUTION: B-FIELD CONFIGURATION

- **Smaller ion flux at the wafer for intermediate cusp locations results in larger overhangs.**

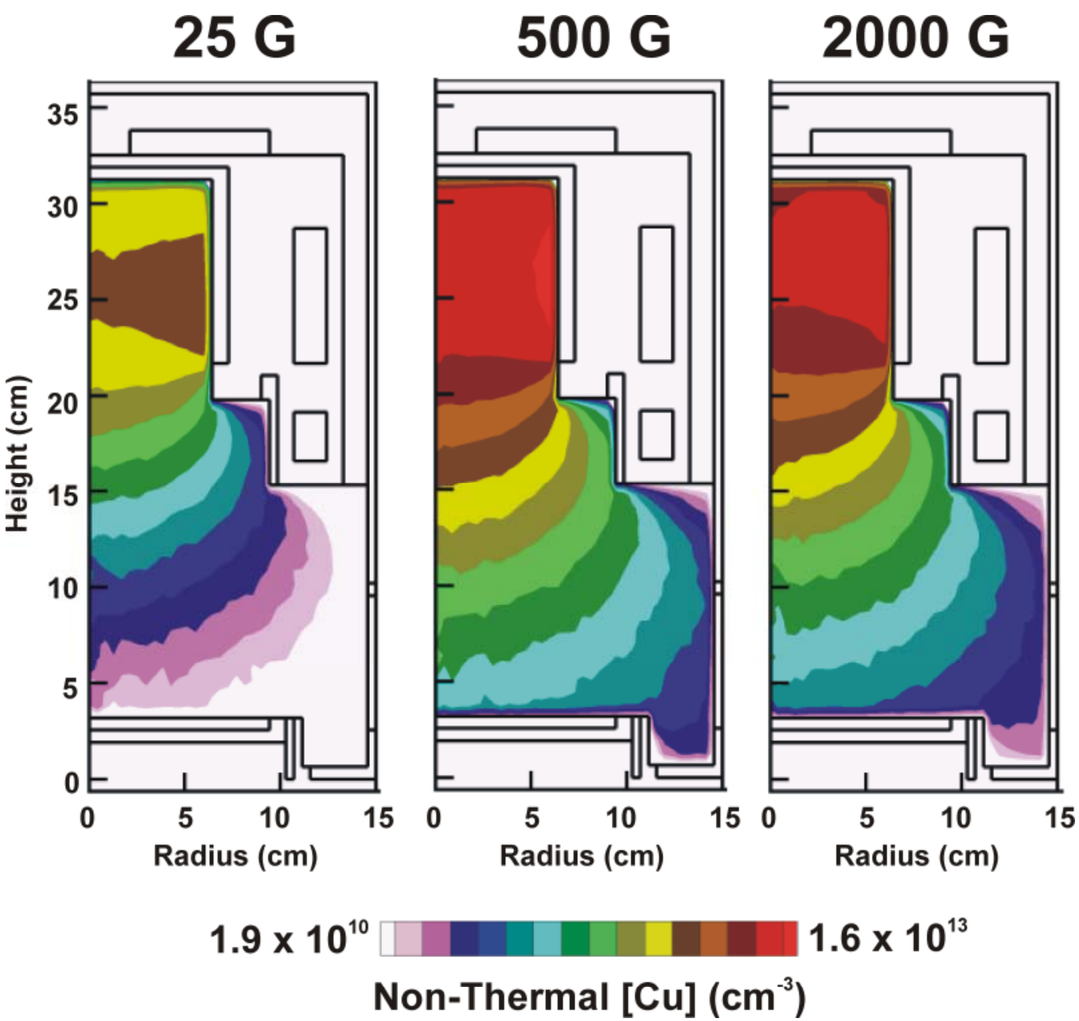


CD = 65 nm, A.R. = 2.5:1

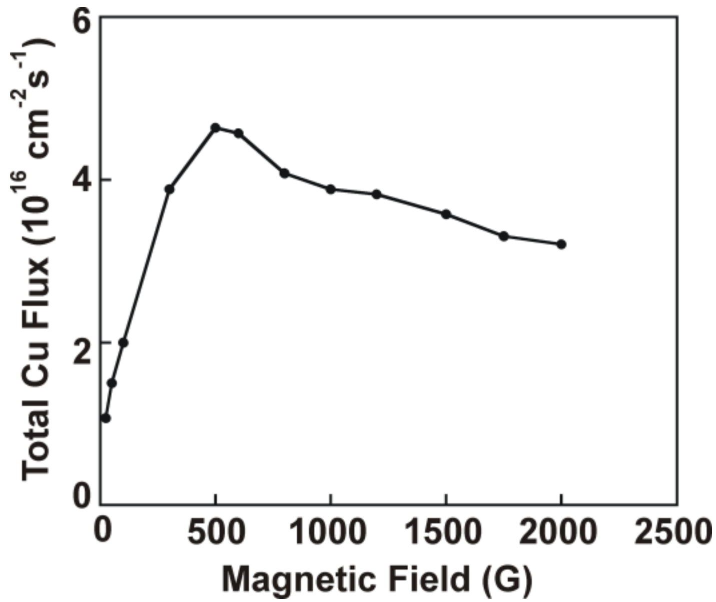
- **10 mTorr, 10 kW**

FLUXES: MAGNETIC FIELD STRENGTH

- The non-thermal [Cu] and total Cu flux onto the substrate increase with B-field upto 500 G; both decrease for higher B-field.



- 10 mTorr, -200 V DC Bias



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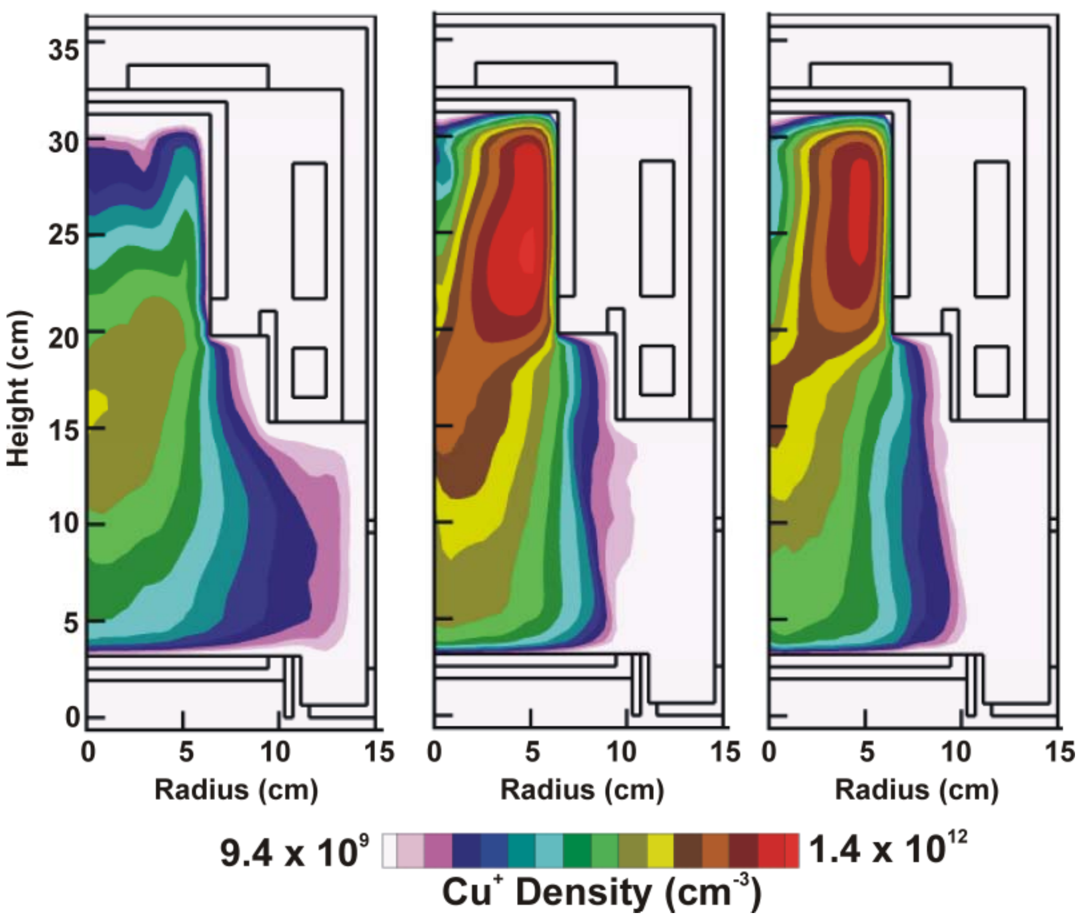
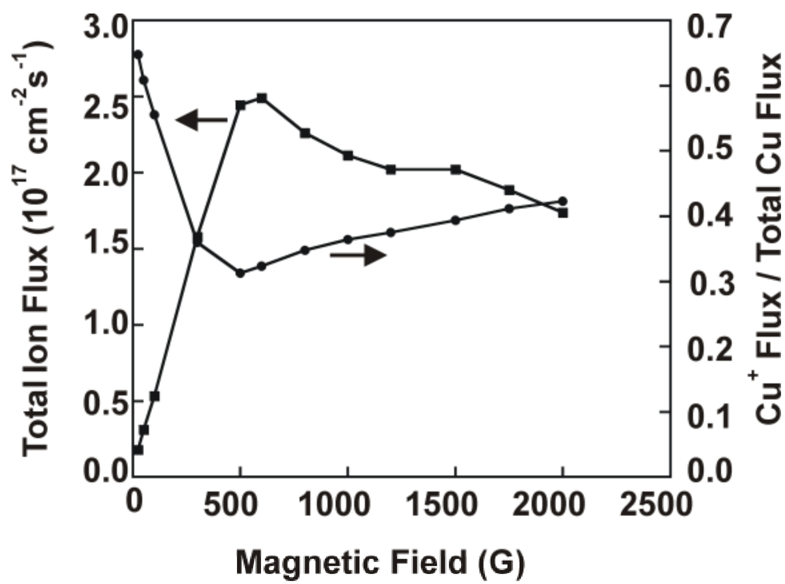
IONIZATION: B-FIELD STRENGTH

- The ion fraction of Cu flux is a minimum for B = 500 G, corresponding to the maximum in non-thermal [Cu] and total ion flux.
- The ionized Cu fraction scales inversely with non-thermal [Cu].



- 10 mTorr, -200 V DC Bias



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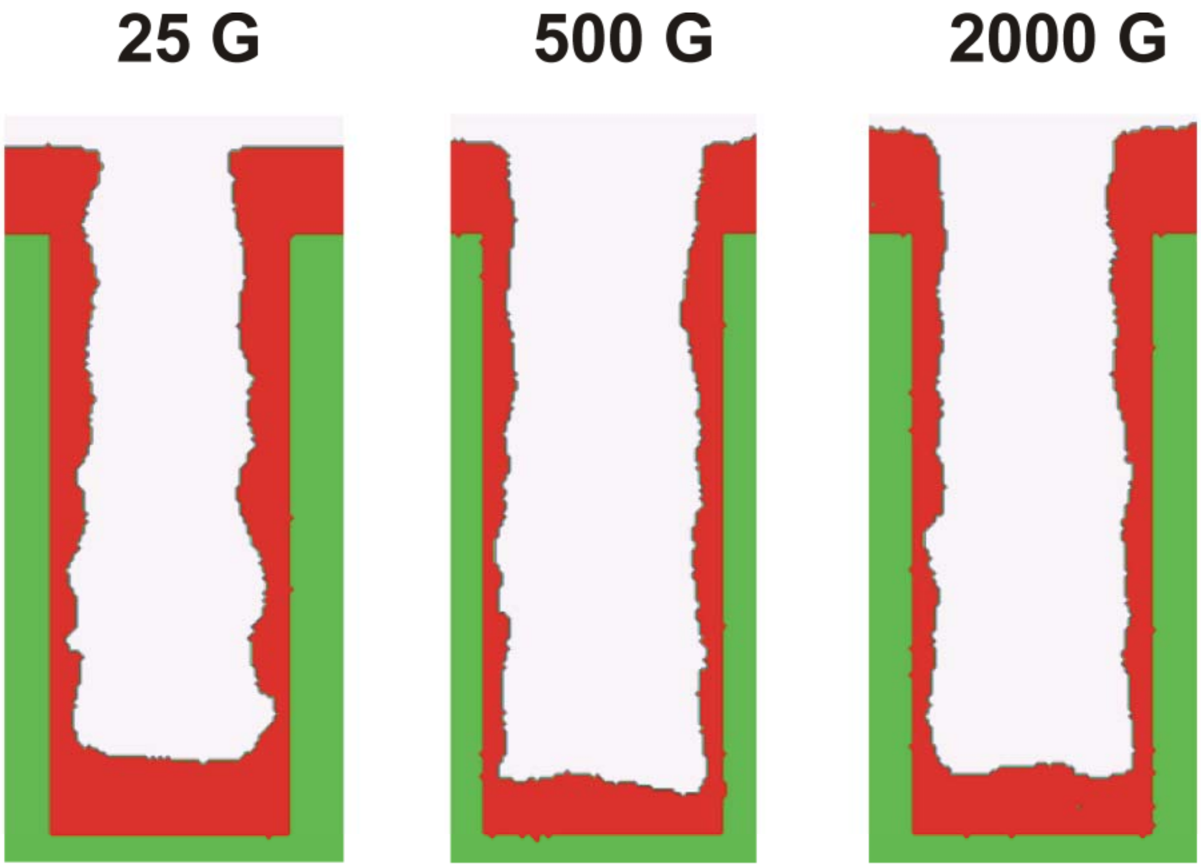
TRENCH EVOLUTION: MAGNETIC FIELD STRENGTH

- **The overhang is maximum for B = 25 G, corresponding to a minimum in total ion flux onto the wafer.**



Overhang: 0.62 **Overhang: 0.34** **Overhang: 0.33**

CD = 65 nm, A.R. = 2.5:1

- **10 mTorr, -200 V DC Bias**

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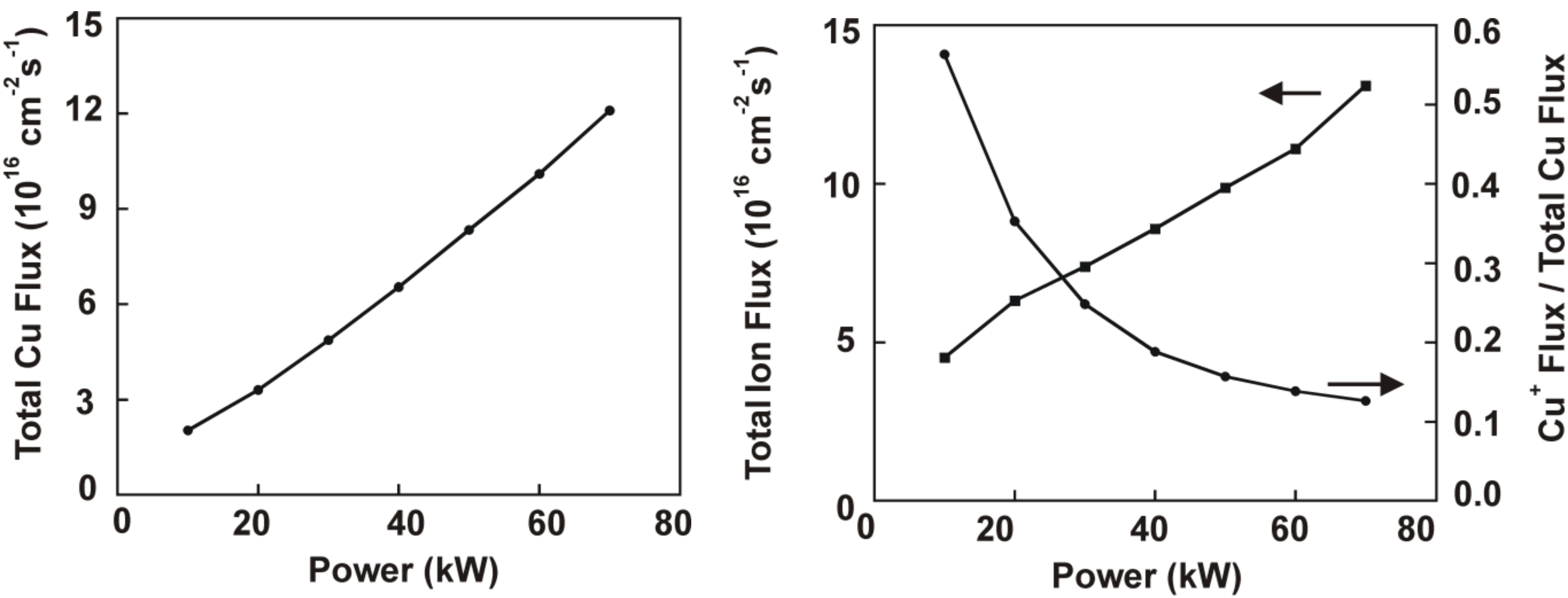
IONIZATION: POWER

- The total Cu flux increases and Cu ion fraction decreases with DC power.

- The total ion flux increases with DC power resulting in a reduced overhang.



- 10 mTorr

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CONCLUDING REMARKS

- A hybrid modeling approach has been developed in which the ion and neutral transport coefficients are kinetically derived and implemented in fluid equations.

- Electron density and sputter densities decrease with decrease in pressure.

- IED's shift to higher energies with decrease in pressure.

- The conditions for maximum ion flux on the wafer were investigated.

- Overhang in Cu seed layer deposition strongly correlates with the total ion flux incident on the wafer.