SOURCES OF NON-EQUILIBRIUM IN PLASMA MATERIALS PROCESSING*

Mark J. Kushner
University of Illinois
Dept. of Electrical and Computer Engineering
1406 W. Green St.
Urbana, IL 61801 USA
mjk@uiuc.edu **http://uigelz.ece.uiuc.edu**

June 2003

* **Work supported by National Science Foundation, Semiconductor Research Corp., Electric Power Research Institute, Applied Materials.**

AGENDA

- Sources of non-equilibrium in plasma processing

- Examples of non-equilibrium

    - Electron transport and electromagnetics
    - Wall chemistry and plasma kinetics
    - Electrostatics in microdischarges

- Concluding Remarks

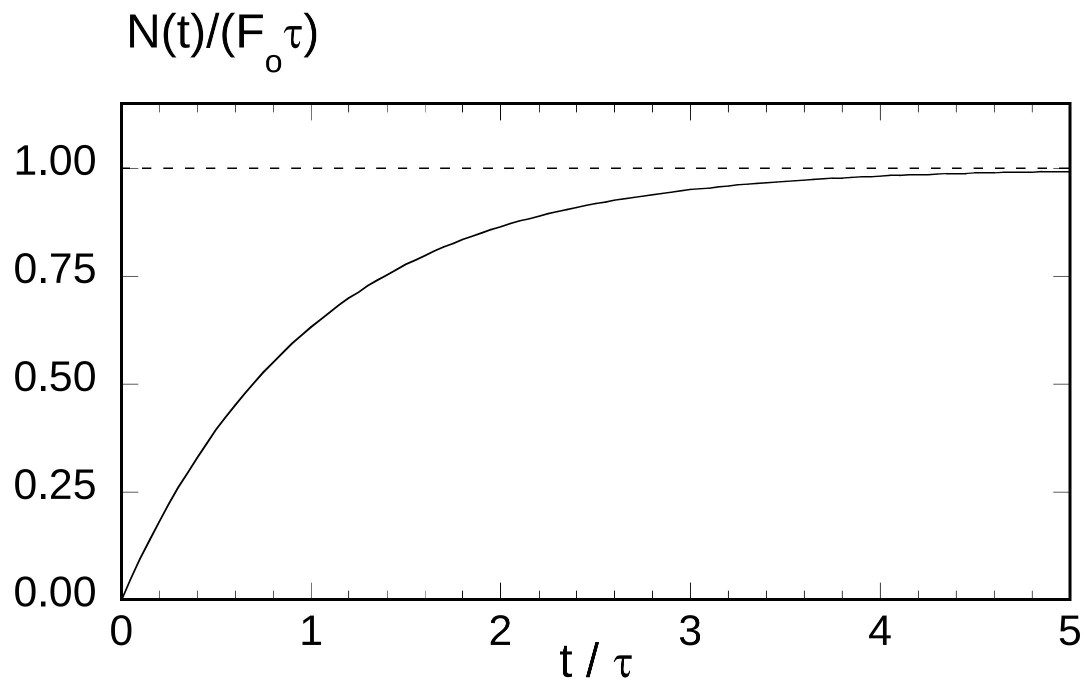
University of Illinois
Optical and Discharge Physics

SO WHAT DO WE MEAN BY (NON-)EQUILIBRIUM?

- **"Non-equilibrium" in plasma processing describes many phenomena, from electron transport to chemical kinetics.**
- **Mathematically…..If *F* is a source function for quantity *N(t)* having damping constant τ, then…**

$$\frac{dN(t)}{dt} = F_o - \frac{N(t)}{\tau}$$

$$N(t) = F_o\tau\left(1 - exp\left(\frac{-t}{\tau}\right)\right)$$



NONEQUILIBRIUM IN ELECTRON TRANSPORT

- **Electron transport is governed by Boltzmann's equation, which describes non-equilibrium evolution of EED in space and time.**

$$\frac{df(\varepsilon,r,t)}{dt} = -\frac{q\vec{E}(r,t)}{m_e}\cdot\nabla_v f(\varepsilon,r,t) - \vec{v}\cdot\nabla f(\varepsilon,r,t) + \left(\frac{\partial f}{\partial t}\right)_c$$

- **Should collisions and advection dominate, spatially dependent steady state time solutions are obtained.**

$$\left|\left(\frac{\partial f}{\partial t}\right)_c\right| \approx \left|\frac{q\vec{E}}{m_e}\cdot\nabla_v f\right| \approx \left|\vec{v}\cdot\nabla f\right| >> \left|\frac{df}{dt}\right|, \quad f = F\big(E(t),N(t)\big)$$

- **Solutions may be adiabatic to slow changes in electric field or densities of collision partners.**

University of Illinois
Optical and Discharge Physics

NONEQUILIBRIUM IN ELECTRON TRANSPORT

- When collisions dissipate energy (and momentum) in distances (or times) small compared to advection, the Local Field approximation is obtained.

$$\left|\left(\frac{\partial f}{\partial t}\right)_c\right| \approx \left|\frac{q\vec{E}}{m_e}\cdot\nabla_v f\right| >> \left|\vec{v}\cdot\nabla f\right|, \quad f(r) = F\left(E(r), N(r)\right)$$

- Non-equilibrium is only manifested by changes in E and N.

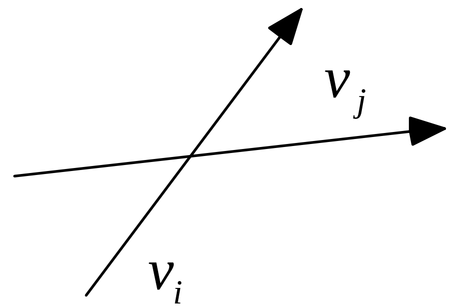
University of Illinois
Optical and Discharge Physics

NONEQUILIBRIUM IN NEUTRAL (ION) TRANSPORT

- **Nonequilibrium in neutral flow often results from "slip" of directed momenta at low pressure .**

$$\frac{\partial N_i}{\partial t} = -\nabla \cdot \phi_i + S_i, \quad \phi_i = \rho_i v_i / m_i$$

$$\frac{\partial(\rho_i v_i)}{\partial t} = -\nabla P_i - \nabla \cdot (\rho_i v_i v_i) - \nabla \cdot \tau - \sum_j f_{ij} \alpha_{ij} (v_i - v_j) + S_i$$



- **If $\alpha_{ij} >> |v/\Delta x|$, the velocities equilibrate and a single fluid results.**

$$\frac{\partial N}{\partial t} = -\nabla \cdot \phi, \quad \phi = \rho v / m, \quad \rho = \sum_i \rho_i$$

$$\frac{\partial(\rho v)}{\partial t} = -\nabla P - \nabla \cdot (\rho v v) - \nabla \cdot \tau + S_i$$

$$\frac{\partial N_i}{\partial t} = -\nabla \cdot \phi_i, \quad \phi_i = N_i v - D_i N_o \nabla \left(\frac{N_i}{N_o} \right)$$

NONEQUILIBRIUM IN CHEMICAL KINETICS

- **Nonequilibrium in chemical kinetics (i.e., the source function) results from reaction rates being slow compared to convection.**

$$\frac{\partial N_i}{\partial t} = -\nabla \cdot \phi_i + S_i$$

$$S_i = -N_i \sum_j N_j k_{ij} + \sum_{j,l} N_j N_l k_{jl} + \left(\nabla \cdot \phi_i\right)\gamma_i - \sum_l \left(\nabla \cdot \phi_l\right)\beta_{il}$$

- **If** $S_i >> N_i\left(v/\Delta x\right)$ **, densities become functions of only local thermodynamic parameters (EOS).**

$$\frac{\partial N_o}{\partial t} = -\nabla \cdot N_o v, \quad N_i = f\left(N_o, T\right)$$

- **Slowly varying boundary conditions such as wall passivation produce long term "nonequilibrium."**

NONEQUILIBRIUM IN ELECTROMAGNETICS

- **Electromagnetics are governed by Maxwell's equations. In the frequency domain,**

$$-\frac{1}{\mu}\left(\nabla\left(\nabla\cdot\overline{E}\right)+\nabla^2\overline{E}\right)=\frac{\partial^2\left(\varepsilon\overline{E}\right)}{\partial t^2}+\overline{J}_{plasma}+\overline{J}_{antenna}$$

- **Although a quasi-steady harmonic state solution, non-equilibrium occurs through the consequences of E on plasma transport.**

$$\nabla\cdot\overline{E}=\rho/\varepsilon_o=0$$ **"Equilibrium"**

$$=\sum_i q_i\int\left(dN_i/dt\right)dt\neq 0$$ **"Nonequilibrium"**

- **These terms most often produce electrostatic waves.**

University of Illinois
Optical and Discharge Physics

NONEQUILIBRIUM IN ELECTROMAGNETICS

- **Nonequilibrium often occurs through the feedback between the E-fields, electron transport and plasma generated current.**

- **Currents which are linearly proportional to fields…equilibrium**

$$\bar{J}_{plasma}(r,t) = \sigma(r,t)\bar{E}(r,t) = \sigma_o(r,t)\bar{E}(r)\exp(i\omega t + \phi(r))$$

- **Currents which have complex relationships to electron (or ion transport) initiated at remote sites…nonequilibrium**

$$\bar{J}_{plasma}(r,t) = \iint G(r,t,r',t')\sigma(r',t')\bar{E}(r',t')dr'\,dt' = \sum_i q_i(N_i v_i)$$

- **In ICP systems, this results in non-monotonic decay of E-fields.**

University of Illinois
Optical and Discharge Physics

ELECTROSTATIC NONEQUILIBRIUM

- **The self shielding of plasmas through the generation of self restoring electric fields provides "electrostatic" equilibrium.**

$$\phi_i = -q_i \mu_i \nabla \Phi - D \nabla N_i \quad \leftrightarrow \quad -\nabla \cdot \varepsilon \nabla \Phi = \sum_i q_i N_i$$

- **Self restoring electric fields ultimately produce quasi-neutrality and ambipolar transport.**

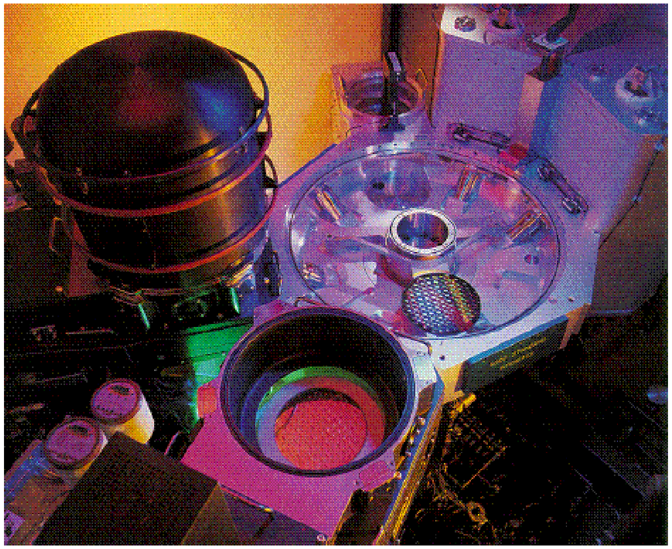
$$\sum_i q_i N_i \approx 0 \quad \rightarrow \quad \phi_i = D_{ambipolar} \nabla N_i$$

- **In systems where dimensions are commensurate with Debye lengths and shielding is incomplete, electrostatic non-equilibrium occurs.**

EXAMPLES OF NON-EQUILIBRIUM

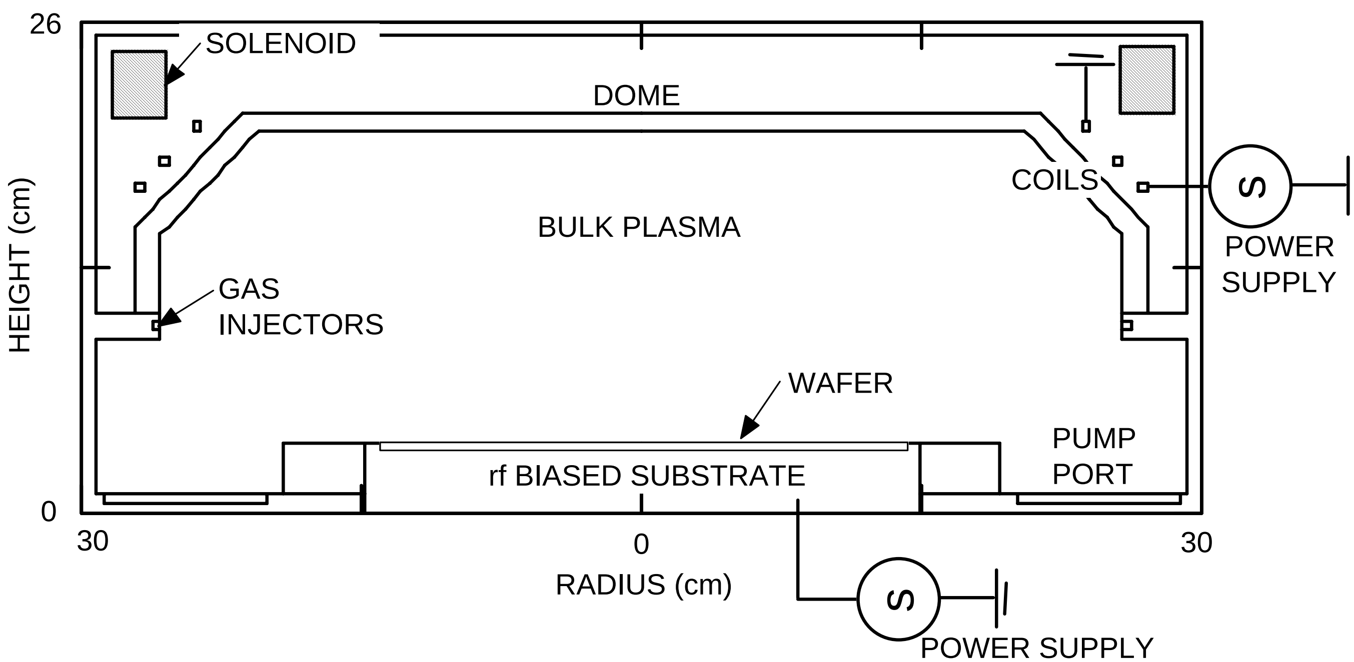
- Electromagnetic non-equilibrium: Anomalous skin depth
- Chemical non-equilibrium: Evolving wall passivation
- Electrostatic nonequilibrium: Microdischarges

University of Illinois
Optical and Discharge Physics



rf BIASED INDUCTIVELY COUPLED PLASMAS

- Inductively Coupled Plasmas (ICPs) with rf biasing are used here.
- < 10s mTorr, 10s MHz, 100s W – kW, electron densities of 10^{11}-10^{12} cm^{-3}.



University of Illinois
Optical and Discharge Physics

ELECTROMAGNETICS MODEL

- **The wave equation is solved in the frequency domain with tensor conductivities.**

$$-\nabla\left(\frac{1}{\mu}\nabla\cdot\overline{E}\right)+\nabla\cdot\left(\frac{1}{\mu}\nabla\overline{E}\right)=\frac{\partial^2\left(\varepsilon\overline{E}\right)}{\partial t^2}+\frac{\partial\left(\overline{\overline{\sigma}}\cdot\overline{E}+\overline{J}\right)}{\partial t}$$

- **The electrostatic term is addressed using a perturbation to the electron density.**

$$\nabla\cdot\overline{E}=\frac{\rho}{\varepsilon}=\frac{q\Delta n_e}{\varepsilon},\quad \Delta n_e=-\nabla\cdot\left(\frac{\overline{\overline{\sigma}}\cdot\overline{E}}{q}\right)/\left(\frac{1}{\tau}+i\omega\right)$$

- **Conduction currents are kinetically derived to account for non-collisional effects.**

$$\mathrm{J}_{\mathrm{e}}\left(\vec{r},t\right)=J_o\left(\vec{r}\right)\exp\left(i\left(\omega t+\phi_v\left(\vec{r}\right)\right)\right)=-qn_e\left(\vec{r}\right)\vec{v}_e\left(\vec{r}\right)\exp\left(i\left(\omega t+\vec{\phi}_v\left(\vec{r}\right)\right)\right)$$

ELECTRON ENERGY TRANSPORT

- **Continuum:**

$$\partial\left(\frac{3}{2}n_e kT_e\right)/\partial t = S(T_e) - L(T_e) - \nabla\cdot\left(\frac{5}{2}\Phi kT_e - \overline{\overline{\kappa}}(T_e)\cdot\nabla T_e\right) + S_{EB}$$

where $S(T_e)$	**=**	**Power deposition from electric fields**
$L(T_e)$	**=**	**Electron power loss due to collisions**
Φ	**=**	**Electron flux**
$\kappa(T_e)$	**=**	**Electron thermal conductivity tensor**
S_{EB}	**=**	**Power source source from beam electrons**

- **Kinetic: A Monte Carlo Simulation is used to derive** $f(\varepsilon, \vec{r}, t)$ **including electron-electron collisions using electromagnetic and electrostatic fields.**

PLASMA CHEMISTRY, TRANSPORT AND ELECTROSTATICS

- **Continuity, momentum and energy equations for each species, and site balance models for surface chemistry.**

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

$$\frac{\partial (N_i \vec{v}_i)}{\partial t} = \frac{1}{m_i} \nabla (k N_i T_i) - \nabla \cdot (N_i \vec{v}_i \vec{v}_i) + \frac{q_i N_i}{m_i} \left(\vec{E} + \vec{v}_i \times \vec{B}\right) - \nabla \cdot \overline{\mu}_i - \sum_j \frac{m_j}{m_i + m_j} N_i N_j (\vec{v}_i - \vec{v}_j) \nu_{ij}$$

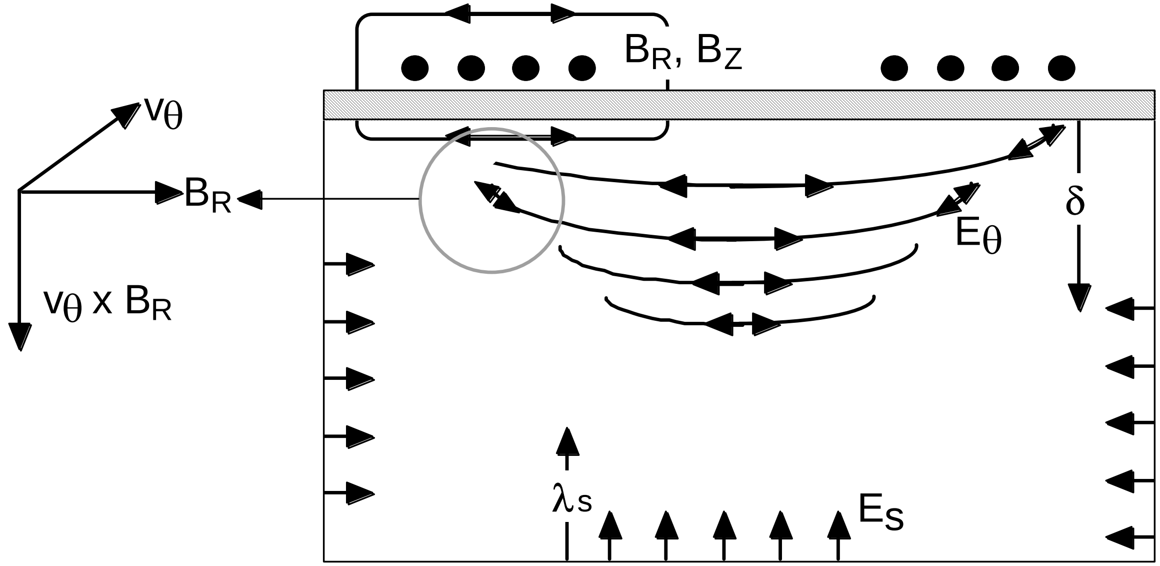
$$\frac{\partial (N_i \varepsilon_i)}{\partial t} + \nabla \cdot \mathrm{Q}_i + P_i \nabla \cdot \mathrm{U}_i + \nabla \cdot (N_i \mathrm{U}_i \varepsilon_i) = \frac{N_i q_i^2 \nu_i}{m_i (\nu_i^2 + \omega^2)} E^2 + \frac{N_i q_i^2}{m_i \nu_i} E_s^2 + \sum_j 3 \frac{m_{ij}}{m_i + m_j} N_i N_j R_{ij} k_B (T_j - T_i) \pm \sum_j 3 N_i N_j R_{ij} k_B T_j$$

- **Implicit solution of Poisson's equation.**

$$\nabla \cdot \varepsilon \nabla \Phi (t + \Delta t) = -\left(\rho_s + \sum_i q_i N_i - \Delta \mathrm{t} \cdot \sum_{\mathrm{i}} \left(\mathrm{q_i} \nabla \cdot \vec{\phi}_i \right) \right)$$

University of Illinois
Optical and Discharge Physics

FORCES ON ELECTRONS IN ICPs



- **Inductive E-field provides azimuthal acceleration; depth 1-3 cm.**

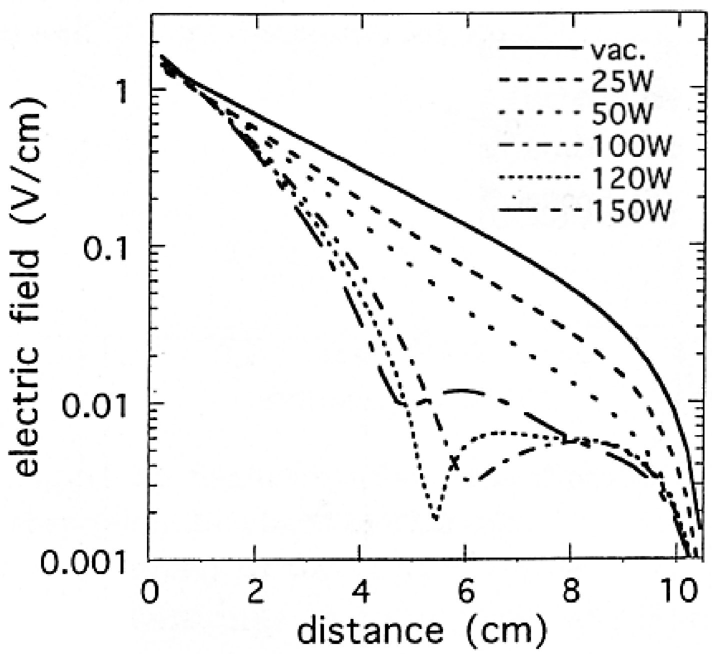
$$\delta = \left(m_e / \left(e^2 \mu_o n_e\right)\right)^{1/2}$$

- **Electrostatic (capacitive) penetrates (100s μm to mm)**

$$\lambda_S \approx 10\lambda_D,\ \lambda_D = \left(kT_e / \left(8\pi n_e e^2\right)\right)^{1/2}$$

- **Non-linear Lorentz Force** $\vec{F} = v_\theta \times \vec{B}_{rf}$

ANAMOLOUS SKIN EFFECT AND POWER DEPOSITION



- Ref: V. Godyak, "Electron Kinetics of Glow Discharges"

- **Collisional heating:**

$$\lambda_{mfp} < \delta_{skin}, \quad \vec{J}_e(\vec{r},t) = \sigma(\vec{r},t)\vec{E}(\vec{r},t)$$

- **Anomalous skin effect:**

$$\lambda_{mfp} > \delta_{skin}$$

$$\vec{J}_e(\vec{r},t) = \iint \sigma(\vec{r},\vec{r}',t,t')\vec{E}(\vec{r}',t')d\vec{r}'dt'$$

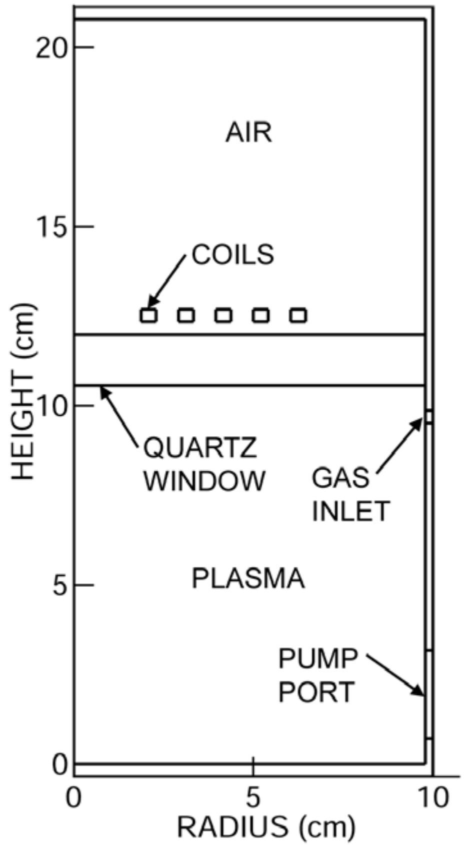
$$\vec{F} = \vec{v} \times \vec{B}$$

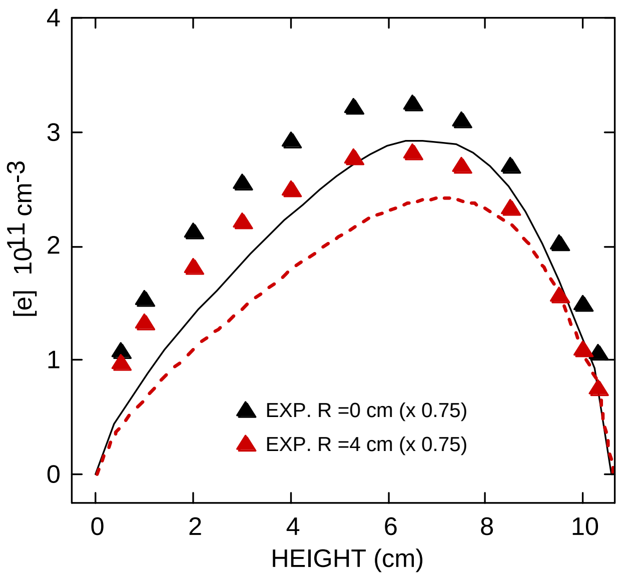
- **Electrons receive (positive) and deliver (negative) power from/to the E-field.**

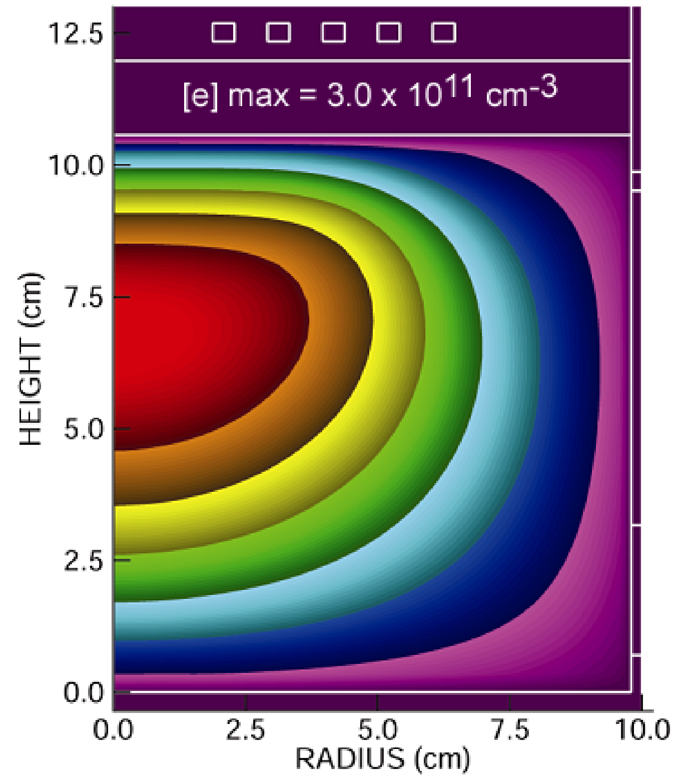
- **E-field is non-monotonic.**

University of Illinois
Optical and Discharge Physics

ELECTRON DENSITY: Ar, 10 mTorr, 200 W, 7 MHz







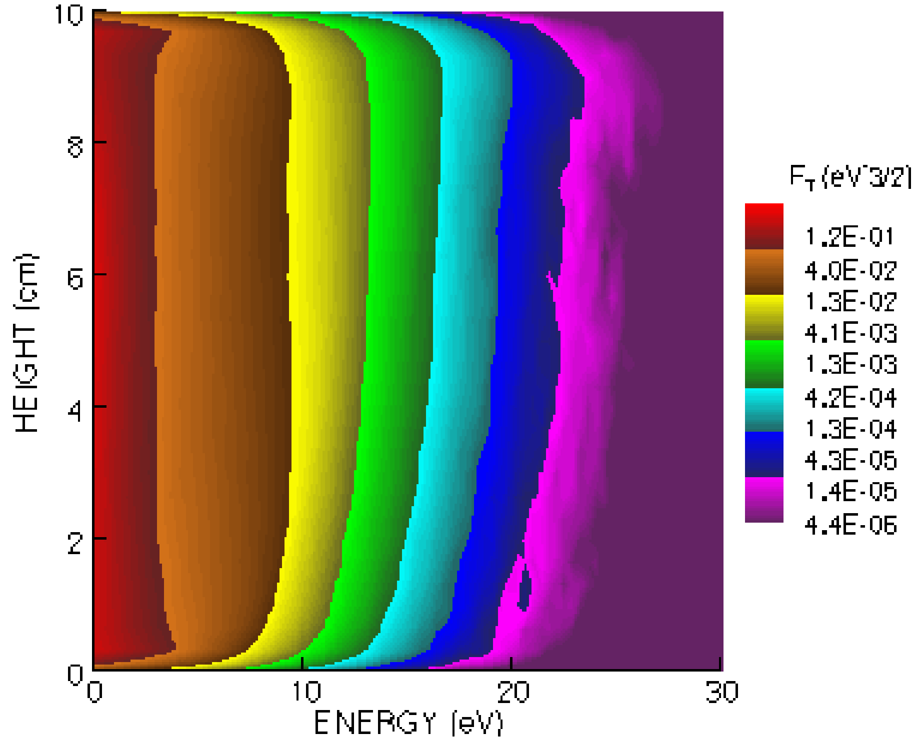
- **Model is about 20% below experiments. This likely has to do with details of the sheath model.**

- **V. Godyak et al, J. Appl. Phys. 85, 703 (1999); private communication**

University of Illinois
Optical and Discharge Physics

TIME DEPENDENCE OF THE EED

- Time variation of the EED is mostly at higher energies where electrons are more collisional.
- Dynamics are dominantly in the electromagnetic skin depth where both collisional and non-linear Lorentz Forces) peak.
- The second harmonic dominates these dynamics.

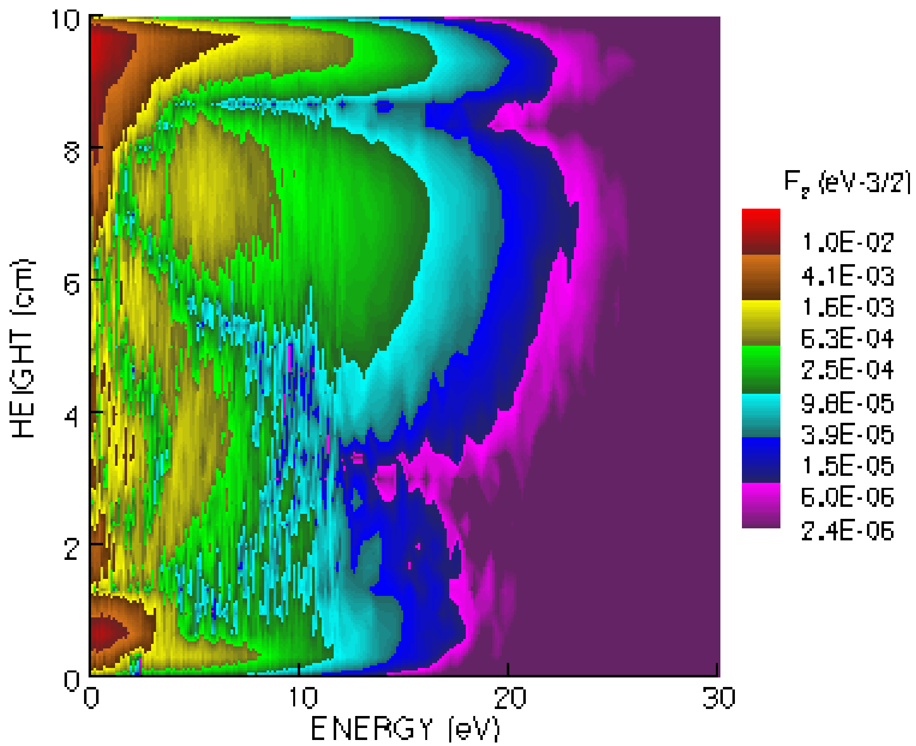


- Ar, 10 mTorr, 100 W, 7 MHz, r = 4 cm

ANIMATION SLIDE

TIME DEPENDENCE OF THE EED: 2nd HARMONIC

- **Electrons in skin depth quickly increase in energy and are "launched" into the bulk plasma.**
- **Undergoing collisions while traversing the reactor, they degrade in energy.**
- **Those surviving "climb" the opposite sheath, exchanging kinetic for potential energy.**
- **Several "pulses" are in transit simultaneously.**
- **Electron transport nonequilibrium!**



- **Amplitude of 2nd Harmonic**

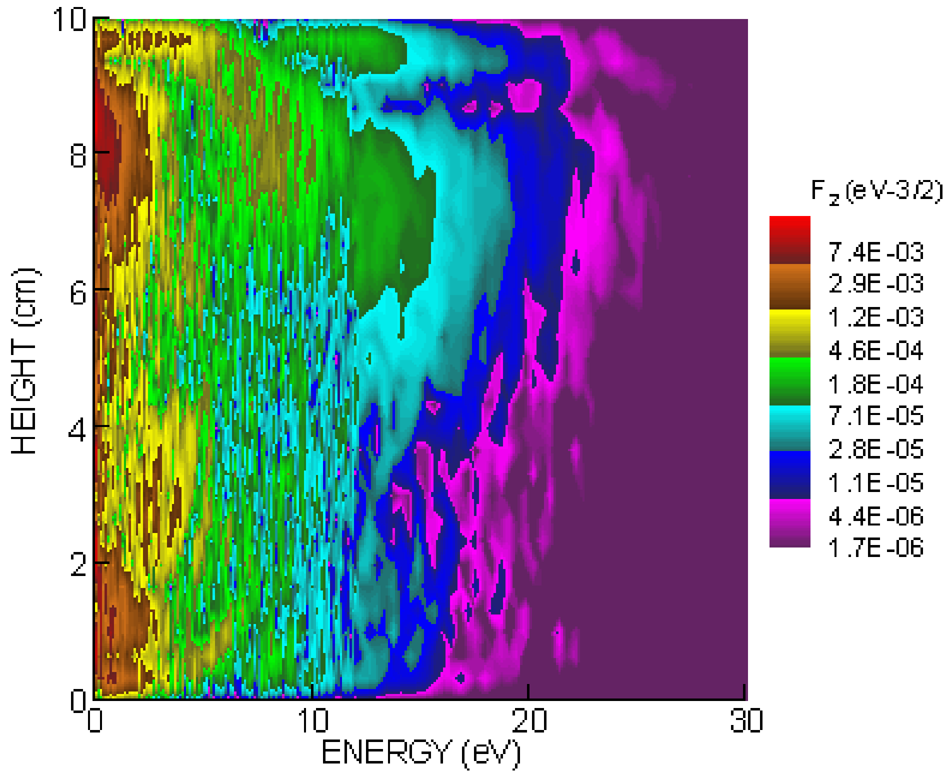
ANIMATION SLIDE

- **Ar, 10 mTorr, 100 W, 7 MHz, r = 4 cm**

University of Illinois
Optical and Discharge Physics

2^{nd} HARMONIC OF EED WITHOUT LORENTZ FORCE

- Excluding v x B terms, the non-linear Lorentz Force is removed.
- Electrons are alternately heated and cooled in the skin depth, out of phase with E_θ, with some collisional heating.
- High energy electrons do not propagate (other than by diffusion) outside the skin layer.



- Amplitude of 2^{nd} Harmonic

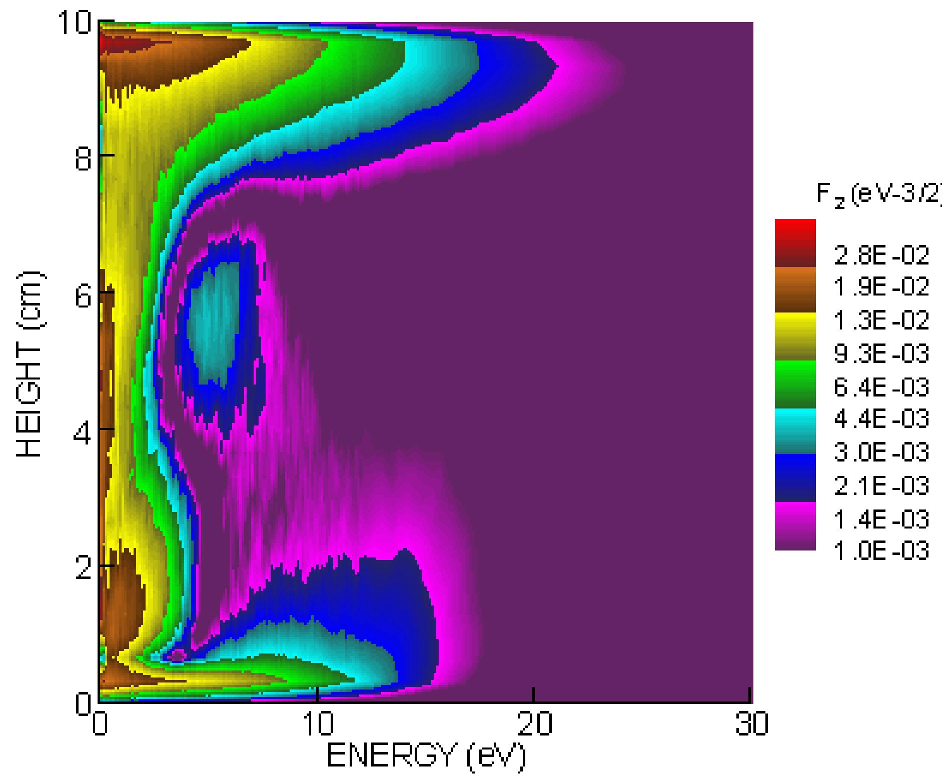
ANIMATION SLIDE

- Ar, 10 mTorr, 100 W, 7 MHz, r = 4 cm

University of Illinois
Optical and Discharge Physics

2^{nd} HARMONIC OF EED: 1 mTorr, 3 MHz

- **By decreasing frequency, B_{rf} increases, the skin depth lengthens and NLF increases.**
- **Lower pressure extends the electron mean free path.**
- **Significant modulation extends to lower energies.**



- **Amplitude of 2^{nd} Harmonic**

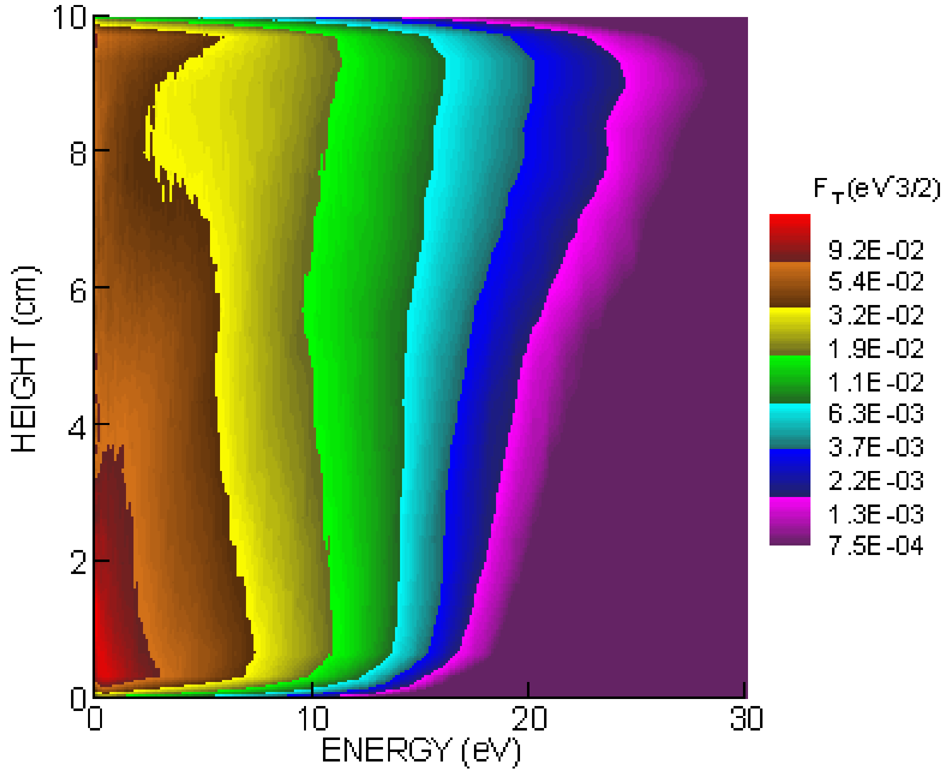
ANIMATION SLIDE

- **Ar, 1 mTorr, 100 W, 3 MHz, r = 4 cm**

University of Illinois
Optical and Discharge Physics

TIME DEPENDENCE OF EED: 1 mTorr, 3 MHz

- **At reduced pressure and frequency, the conditions for the nonlinear skin effect are fulfilled.**
- **The EED is essentially depleted of low energy electrons in the skin layer.**

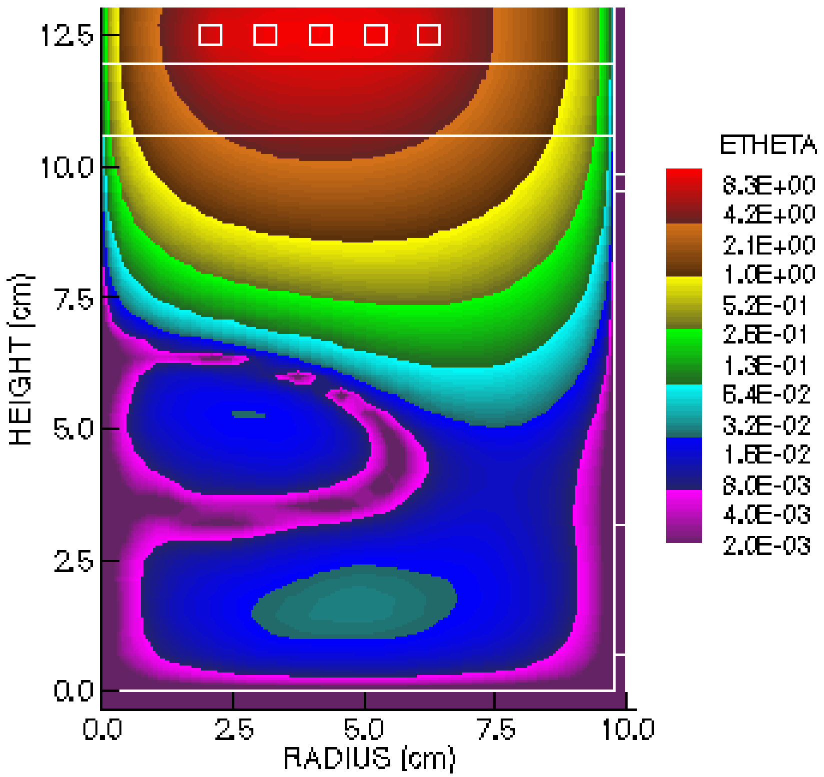


ANIMATION SLIDE

- **Ar, 1 mTorr, 100 W, 3 MHz, r = 4 cm**

COLLISIONLESS TRANSPORT ELECTRIC FIELDS

- E_θ exhibits extrema and nodes resulting from this non-collisional transport.
- "Sheets" of electrons with different phases provide current sources interfering or reinforcing the electric field for the next sheet.
- Axial transport results from $\vec{v} \times \vec{B}_{rf}$ forces.
- **Electromagnetic nonequilibrium!**

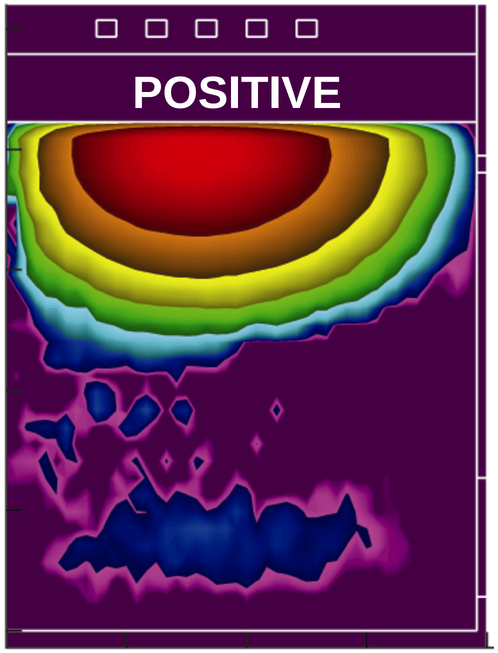


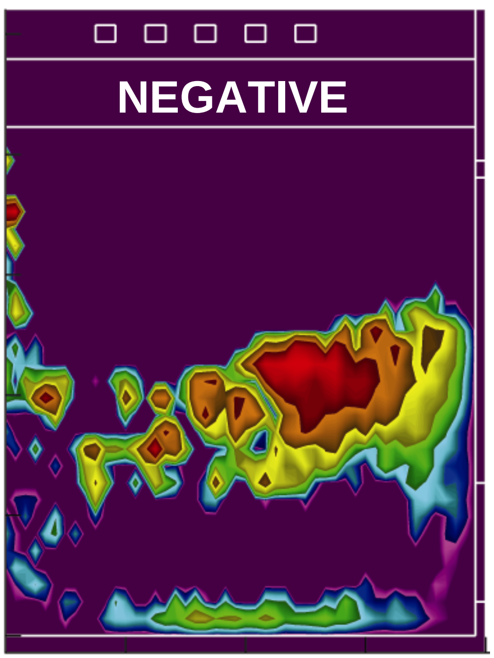
ANIMATION SLIDE

- Ar, 10 mTorr, 7 MHz, 100 W

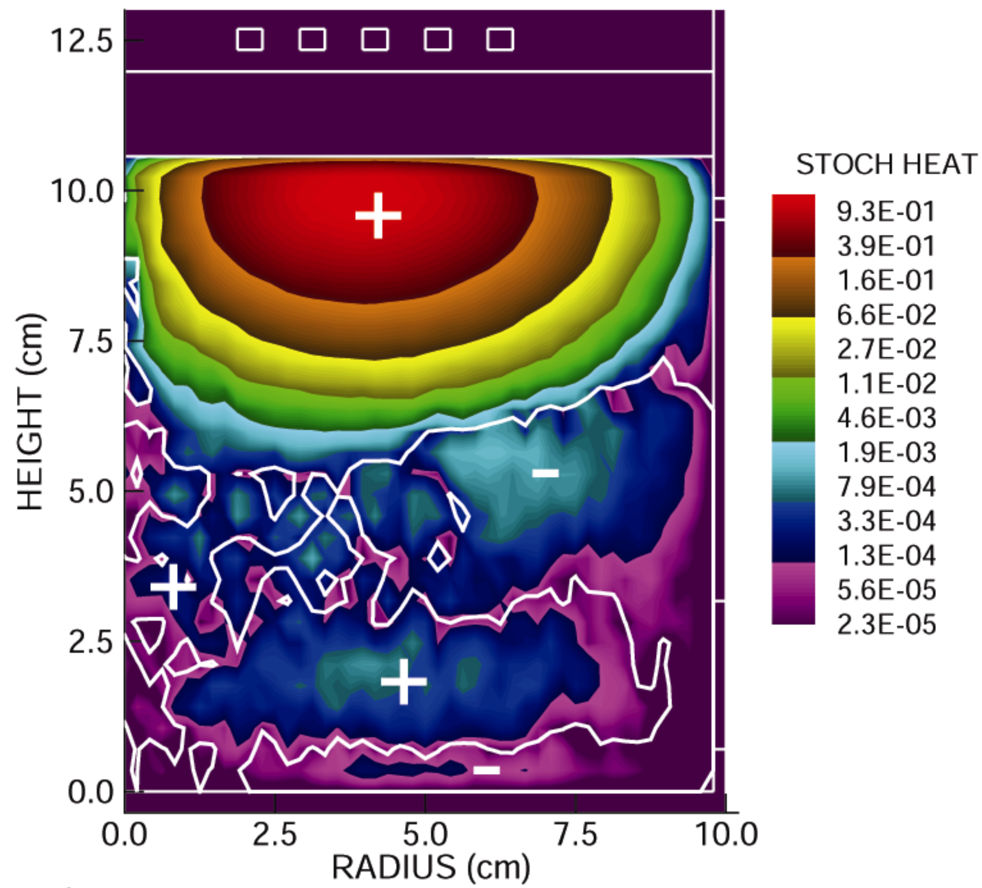
University of Illinois
Optical and Discharge Physics

POWER DEPOSITION: POSITIVE AND NEGATIVE





- The end result is regions of positive and negative power deposition.

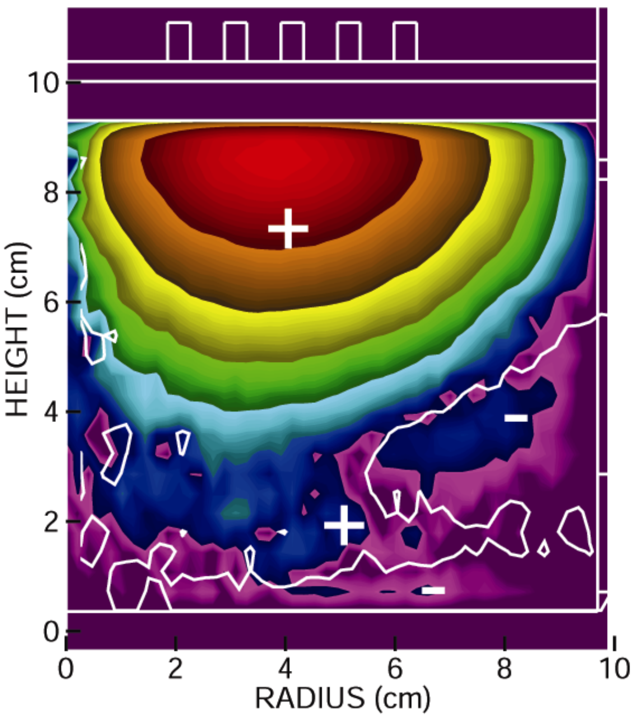


- Ar, 10 mTorr, 7 MHz, 100 W

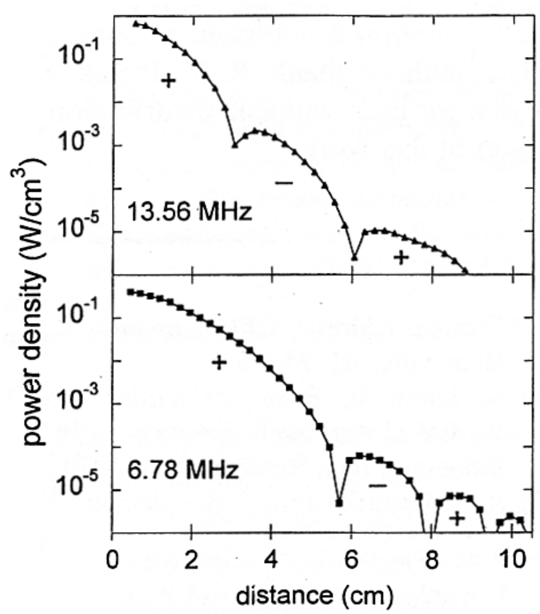
University of Illinois
Optical and Discharge Physics

POWER DEPOSITION vs FREQUENCY

- **The shorter skin depth at high frequency produces more layers of negative power deposition of larger magnitude.**

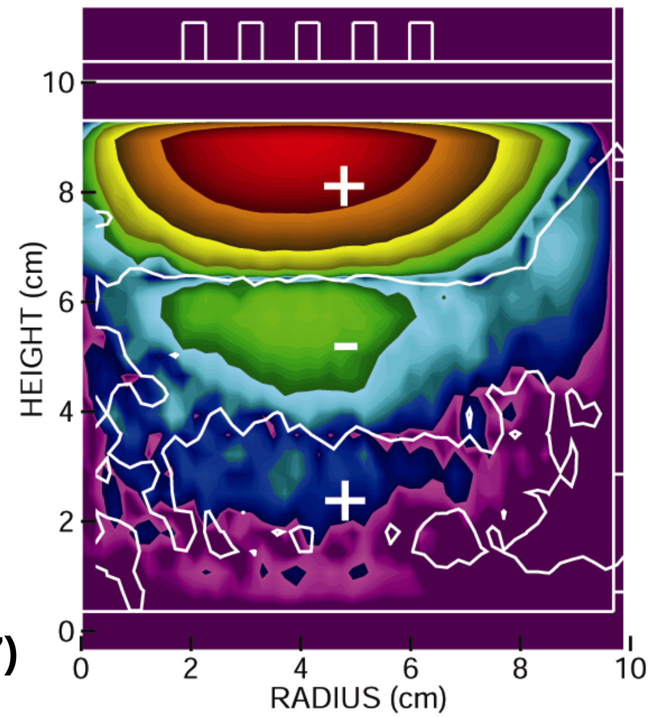


• 6.7 MHz
(5x10^{-5} – 1.4 W/cm^3)

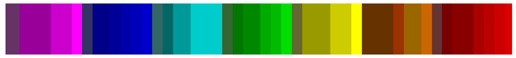


- **Ref: Godyak, PRL (1997)**

- **Ar, 10 mTorr, 200 W**



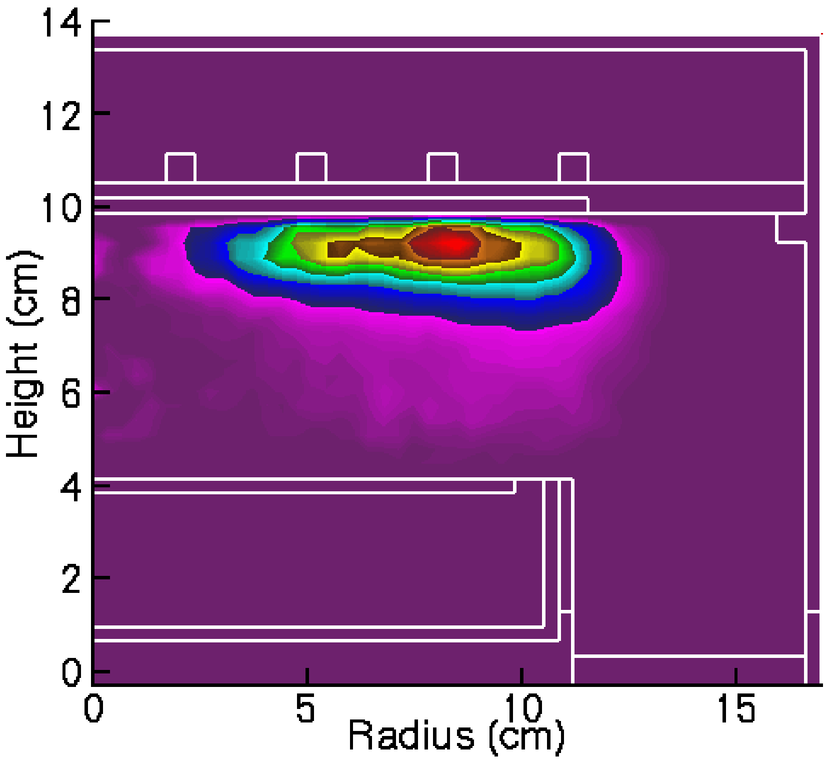
• 13.4 MHz
(8x10^{-5} – 2.2 W/cm^3)

MIN  **MAX**

University of Illinois
Optical and Discharge Physics

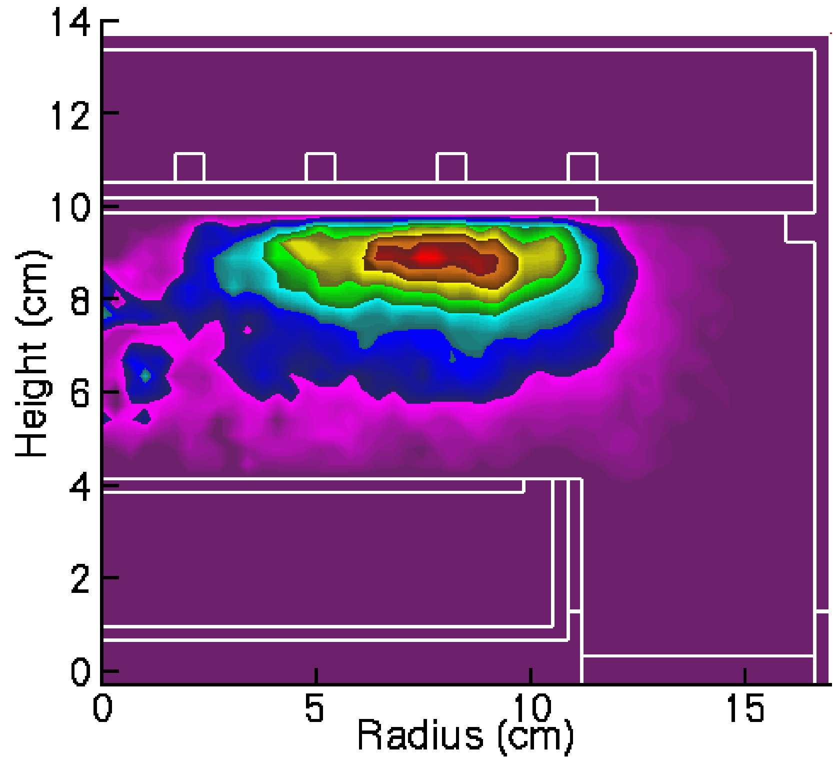
TIME DEPENDENCE OF Ar IONIZATION: PRESSURE

- Although B_{rf} may be nearly the same, at large P, v_θ and mean-free-paths are smaller, leading to lower harmonic amplitudes.



- 5 mTorr

$6 \times 10^{14} – 3 \times 10^{16}$ $cm^{-3}s^{-1}$



- 20 mTorr

$1.5 \times 10^{14} – 1.7 \times 10^{16}$ $cm^{-3}s^{-1}$

- Ar/N_2=60/40, 10 MHz

ANIMATION SLIDE

MIN MAX

SNLA_0102_29

University of Illinois
Optical and Discharge Physics

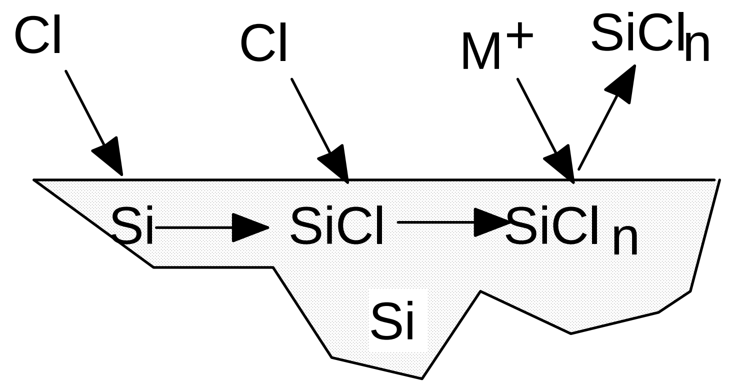
EXAMPLES OF NON-EQUILIBRIUM

- Electromagnetic non-equilibrium: Anomalous skin depth
- Chemical non-equilibrium: Evolving wall passivation
- Electrostatic nonequilibrium: Microdischarges

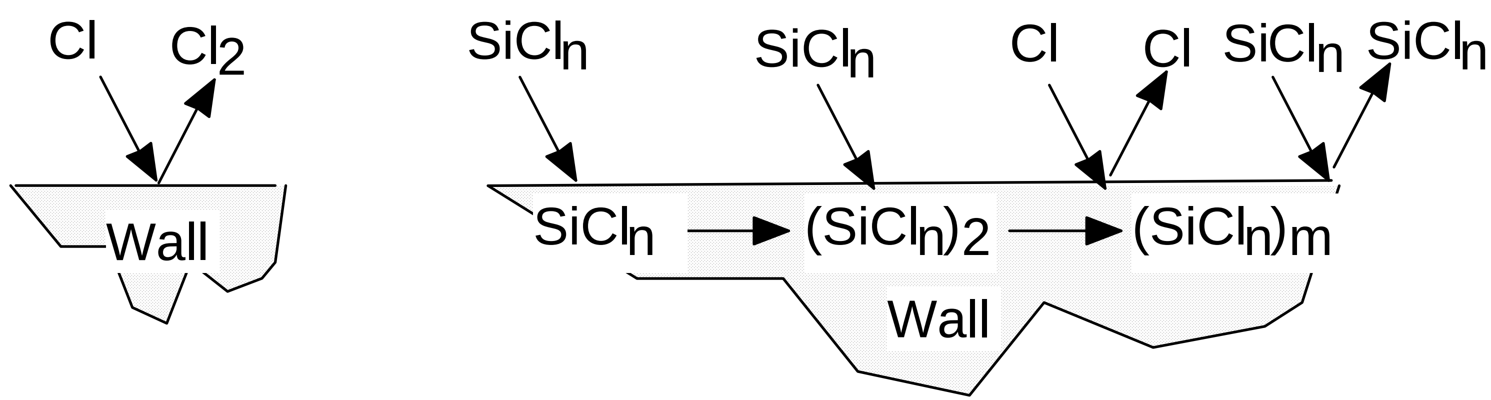
University of Illinois
Optical and Discharge Physics

SURFACE CHEMISTRY OF Si ETCHING IN Cl_2 PLASMAS

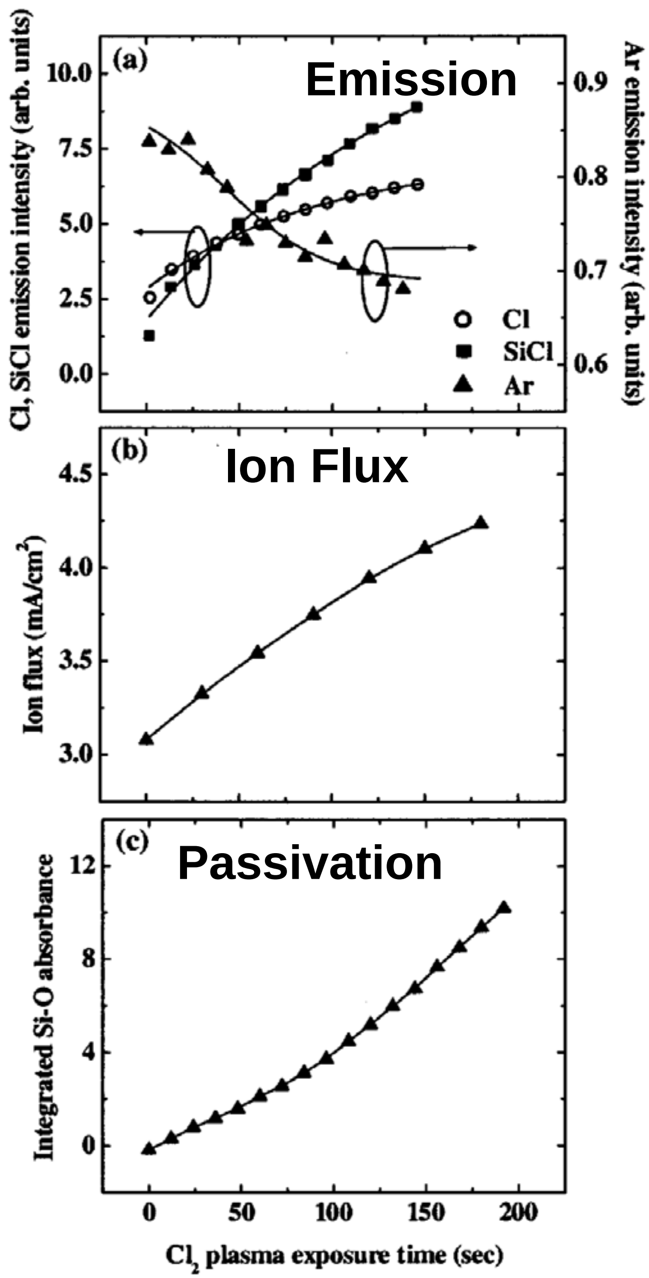
- **Etching of Si in Cl_2 plasmas proceeds by passivation of Si sites, followed by ion activated removal of $SiCl_n$ etch product .**



- **Etch products deposit on reactor walls. Cl atom recombination and $SiCl_n$ sticking slows on the passivated surfaces.**



University of Illinois
Optical and Discharge Physics



LONG TERM PASSIVATION OF WALLS

- **Experimental measurements of optical emission, ion flux and etch rates during Cl etching of Si have long term behavior.**
- **Transients are correlated with increasing film thickness on walls, reducing sticking coefficients for Cl and SiCl.**
- **ICP, Cl_2, 10 mTorr, 800 W.**
- **Plasma-surface chemical nonequilibrium!**
- **S. J. Ullal, T. W. Kim, V. Vahedi and E. S. Aydil, JVSTA 21, 589 (2003)**

CHEMICAL NONEQUILIBRIUM: Ar/Cl_2 WITH WALL PASSIVATION

- **Computationally contrast Ar/Cl_2 ICPs etching Si with $SiCl_2$ product, with/without wall passivation.**

- **Implement a multistep passivation model beginning with $SiCl_2$ polymerization. Higher degree of polymerization reduces Cl reassociation.**

- **Without wall passivation:** $Cl \rightarrow wall \rightarrow Cl_2$, $p = 0.3$

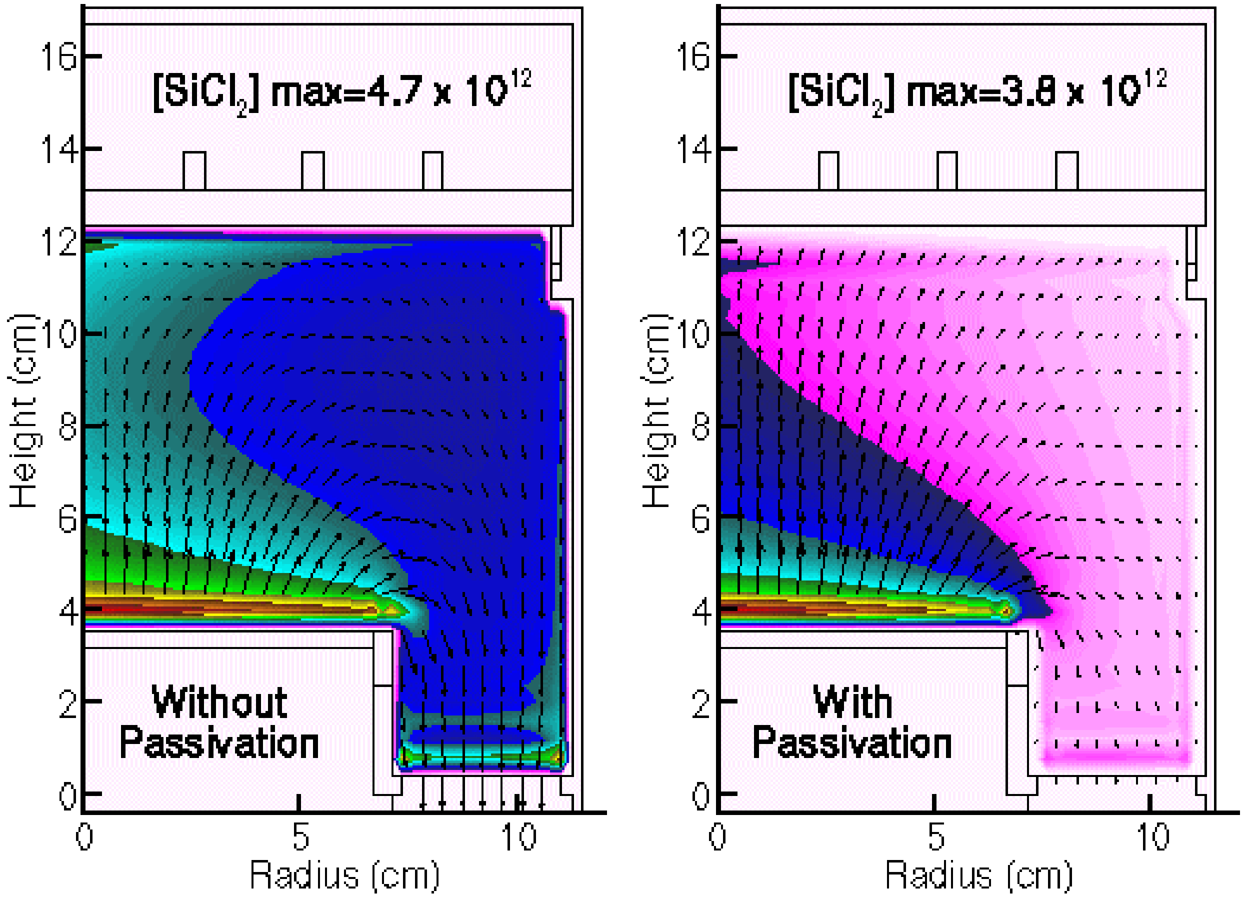
- **With final wall passivation:** $Cl \rightarrow wall \rightarrow Cl_2$, $p = 0.01$

- **Ar/Cl_2 = 80/20, 10 mTorr, 400 W, 200 sccm**

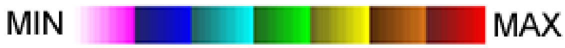
University of Illinois
Optical and Discharge Physics

[$SiCl_2$] WITH/WITHOUT WALL PASSIVATION

- Without passivation, $SiCl_2$ has a longer residence time and builds to higher densities. Note momentum transfer from jetting nozzle.



- Ar/Cl_2 = 80/20, 10 mTorr, 400 W, 200 sccm

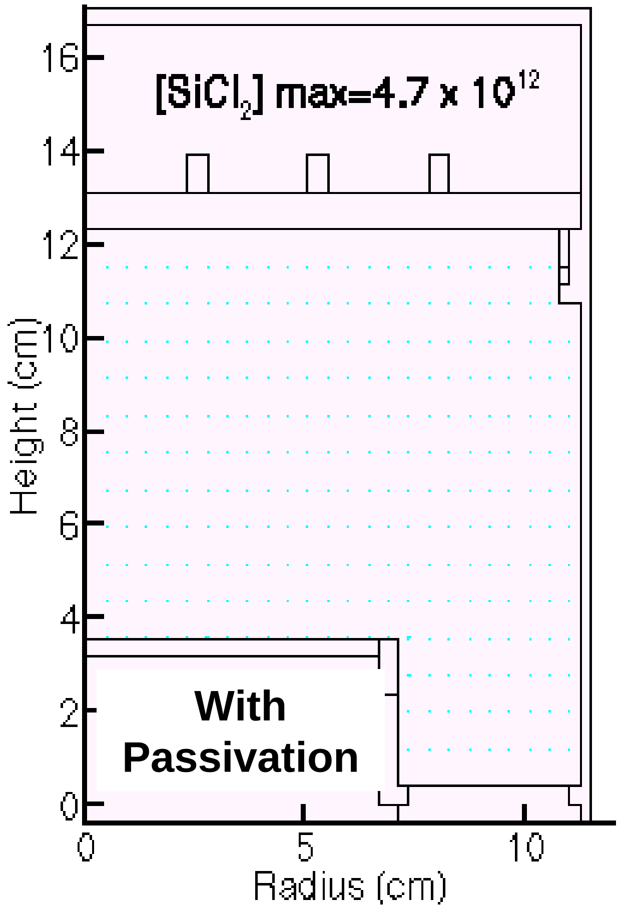


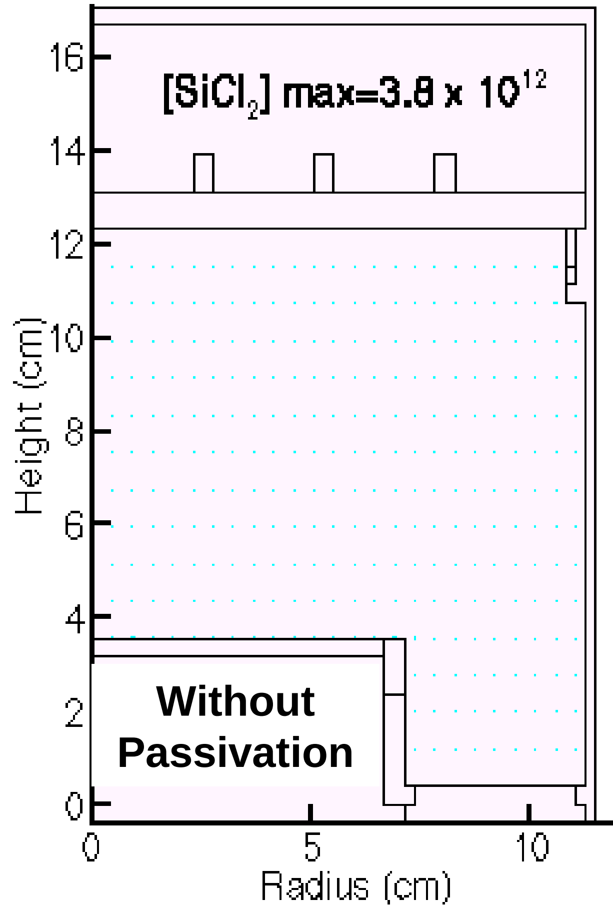
ISPC03_21

University of Illinois
Optical and Discharge Physics

[$SiCl_2$] TRANSIENT WITH/WITHOUT WALL PASSIVATION

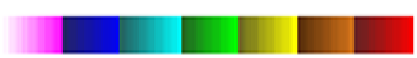
- **$SiCl_2$ initially sticks to walls in both cases. As passivation progresses, the sticking coefficient decreases.**





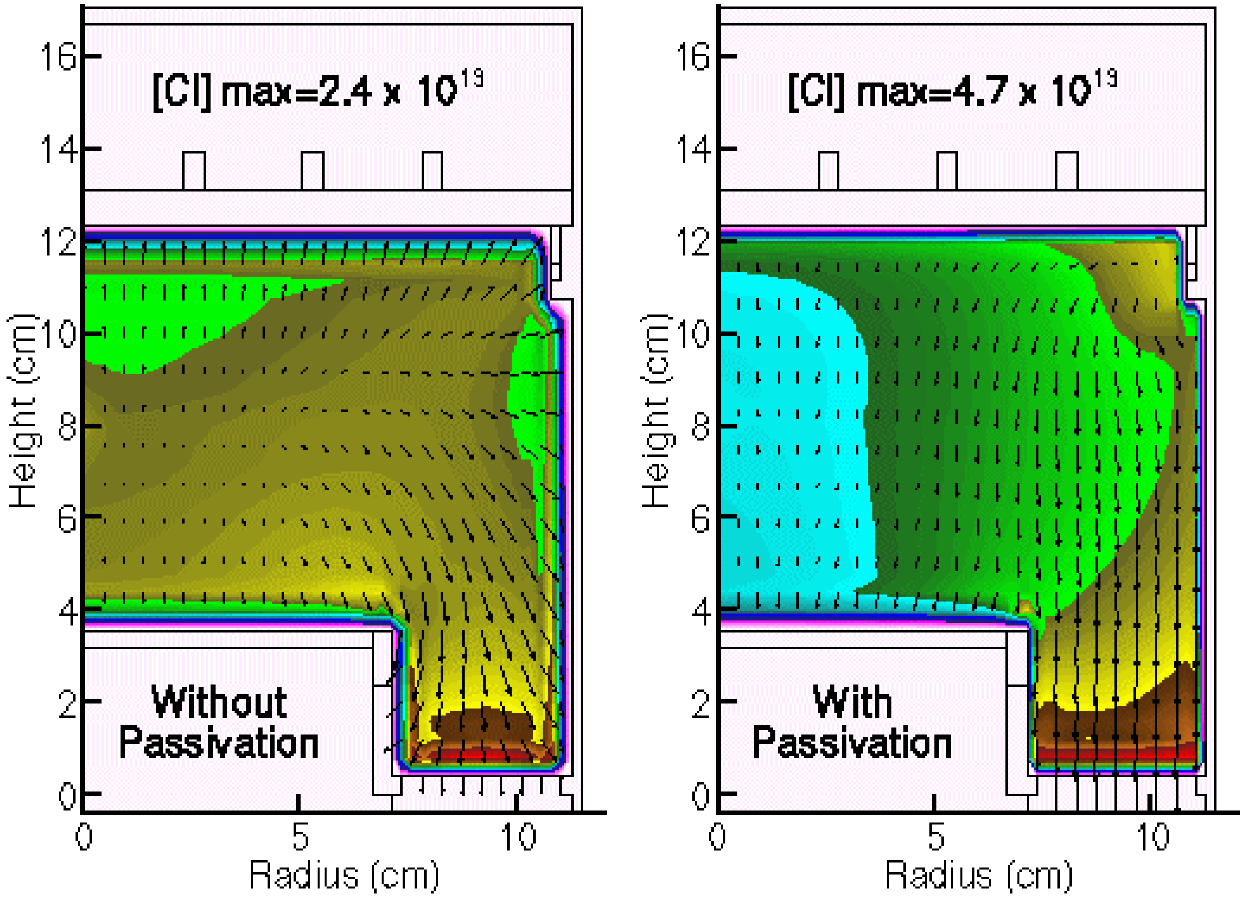
ANIMATION SLIDE

- **Ar/Cl_2 = 80/20, 10 mTorr, 400 W, 200 sccm**



[Cl] WITH/WITHOUT WALL PASSIVATION

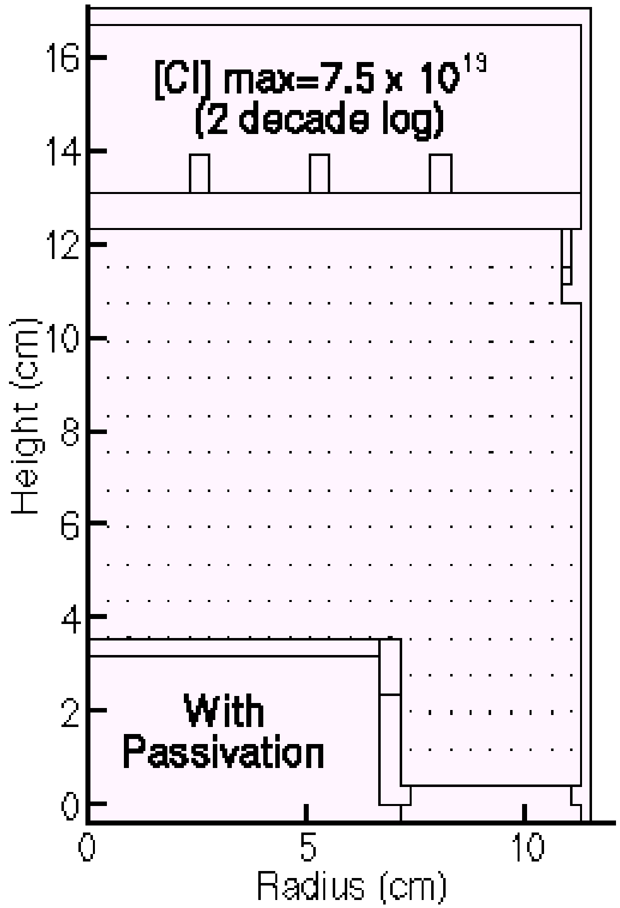
- **Passivation reduces Cl losses on the walls, increasing its density and making pumping the largest loss.**



- **Ar/Cl_2 = 80/20, 10 mTorr, 400 W, 200 sccm**

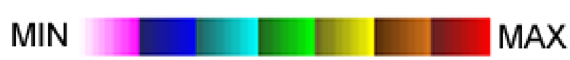
[Cl] TRANSIENT WITH WALL PASSIVATION

- **When walls are clean, Cl reassociation is a large sink. As the walls passivate, surface losses decrease (except to wafer).**



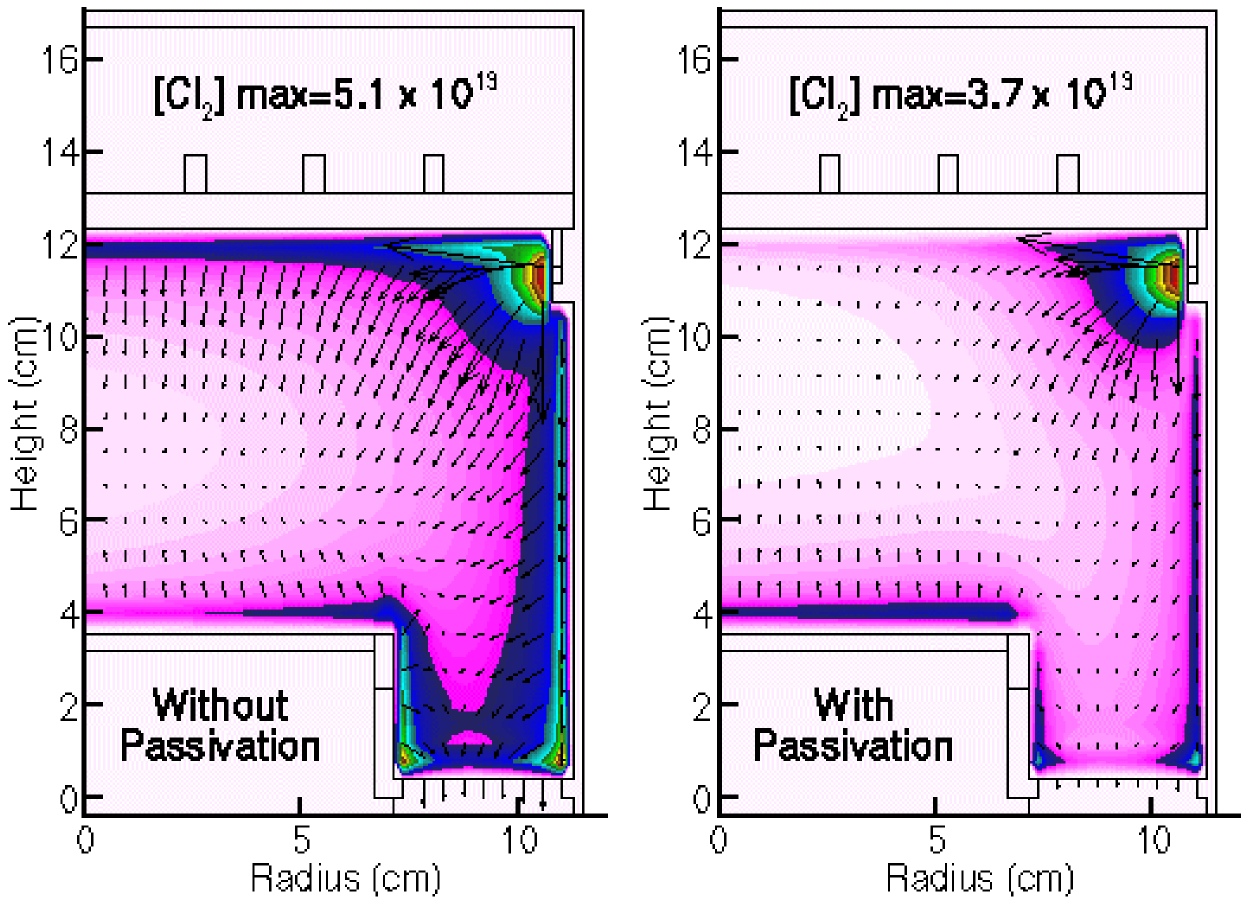
ANIMATION SLIDE

- **Ar/Cl_2 = 80/20, 10 mTorr, 400 W, 200 sccm**

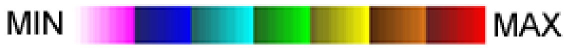


[Cl_2] WITH/WITHOUT WALL PASSIVATION

- **Without passivation, Cl_2 has sources at walls, raising its density. In both cases, dissociation fraction is large.**



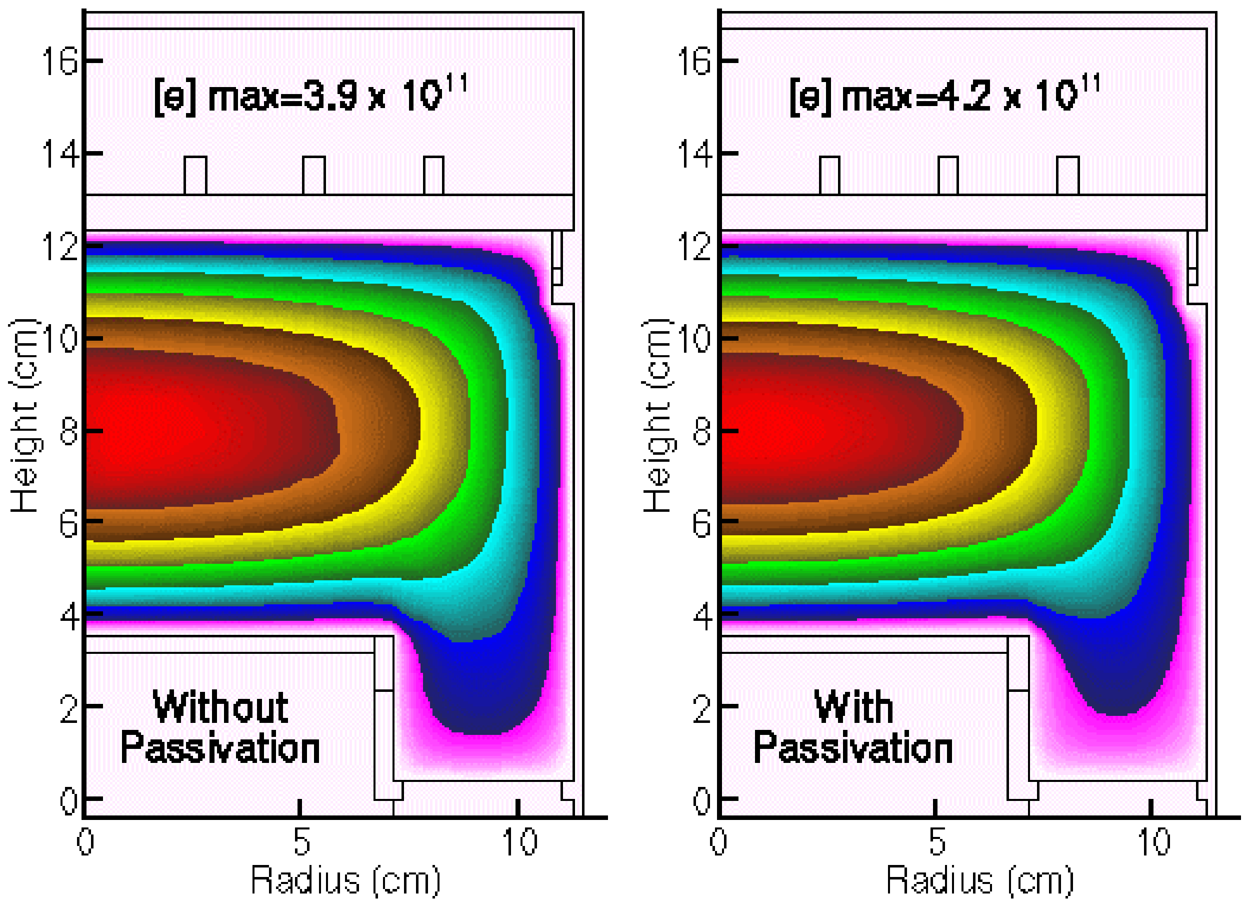
- **Ar/Cl_2 = 80/20, 10 mTorr, 400 W, 200 sccm**



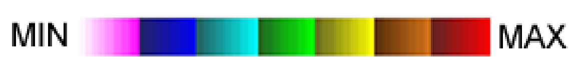
University of Illinois
Optical and Discharge Physics

[e] WITH/WITHOUT WALL PASSIVATION

- Without wall passivation, sources Cl_2 from the walls are larger, resulting in more dissociative attachment and lower [e].



- Ar/Cl_2 = 80/20, 10 mTorr, 400 W, 200 sccm



University of Illinois
Optical and Discharge Physics

EXAMPLES OF NON-EQUILIBRIUM

- Electromagnetic non-equilibrium: Anomalous skin depth
- Chemical non-equilibrium: Evolving wall passivation
- Electrostatic non-equilibrium: Microdischarges

University of Illinois
Optical and Discharge Physics

MICRODISCHARGE PLASMA SOURCES

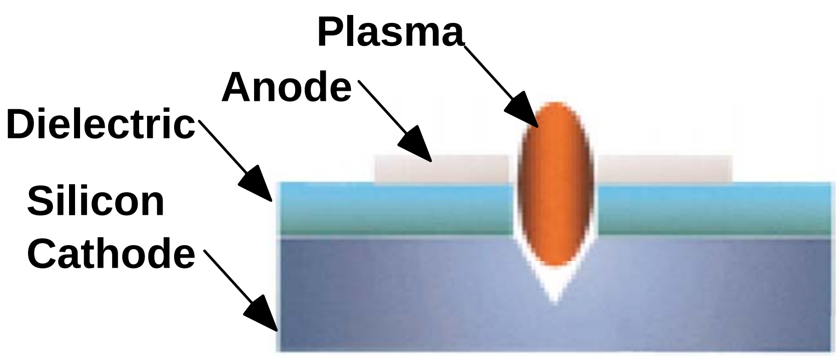
- **Microdischarges are plasma devices which leverage pd scaling to operate dc atmospheric glows 10s –100s μm in size.**
- **MEMS fabrication techniques enable innovative structures for displays and detectors.**
- **Although similar to PDP cells, MDs are dc devices which largely rely on nonequilibrium beam components of the EED.**
- **Electrostatic nonequilibrium results from their small size. Debye lengths and cathode falls are commensurate with size of devices.**

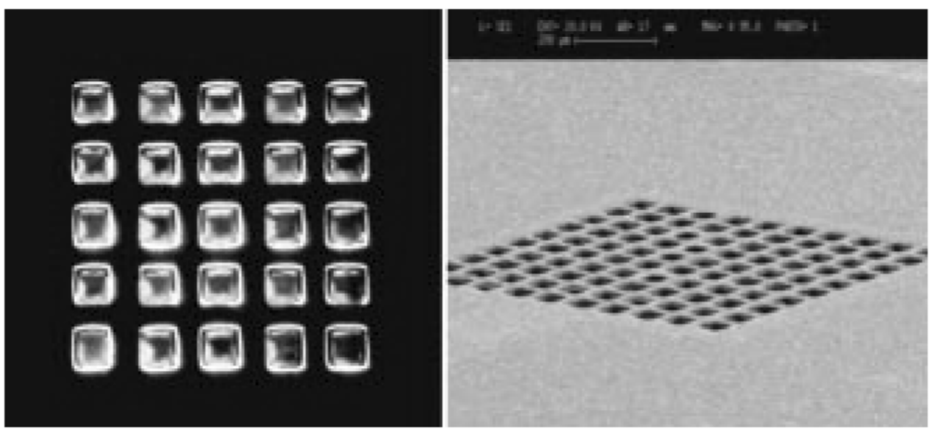
$$L_{cathodeFall} = \left(2V_c\varepsilon_0 / \left(qn_I\right)\right)^{1/2} \approx 10 - 20\mu m$$

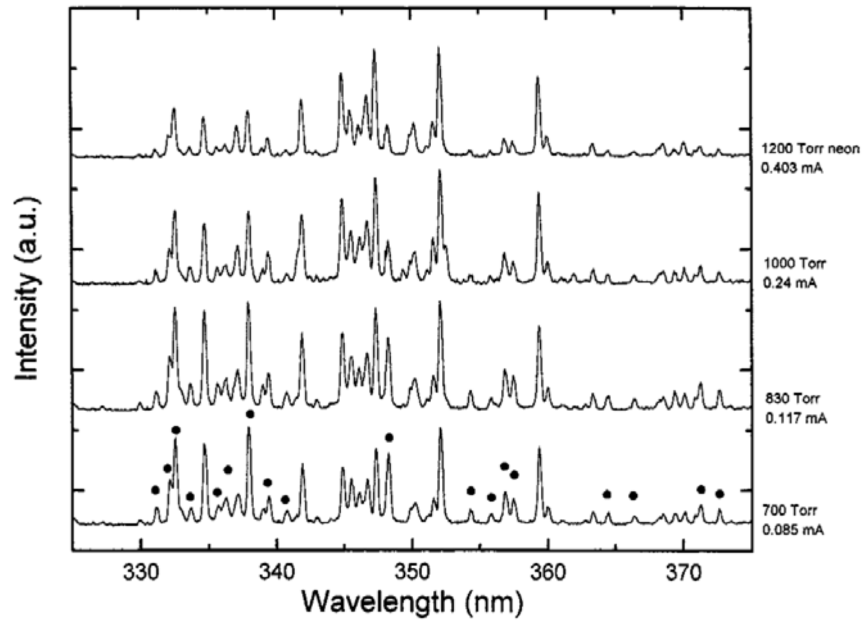
$$\lambda_D \approx 750\left(\frac{T_{eV}}{n_e(cm^{-3})}\right)^{1/2} cm \approx 10\mu m,$$

PYRAMIDAL MICRODISCHARGE DEVICES

- Si MDs with 10s μm pyramidal cavities display nonequilibrium behavior: Townsend to negative glow transitions.
- Small size also implies electrostatic nonequilibrium.







- S.-J. Park, et al., J. Sel. Topics Quant. Electron 8, 387 (2002); Appl. Phys. Lett. 78, 419 (2001).

2-D MODELING OF MICRODISCHARGE SOURCES

- **Charged particle continuity (fluxes by Sharfetter-Gummel form)**

$$\frac{\partial N_i}{\partial t} = -\vec{\nabla} \cdot \left(qN_i \mu_i \left(-\vec{\nabla}\Phi \right) - D_i \nabla N_i \right) + S_i$$

- **Poisson's Equation for Electric Potential**

$$-\nabla \cdot \varepsilon \nabla \Phi = \rho_V + \rho_S$$

- **Bulk continuum electron energy transport and MCS beam.**

$$\frac{\partial (n_e \varepsilon)}{\partial t} = \vec{j} \cdot \vec{E} - n_e \sum_i N_i \kappa_i - \nabla \cdot \left(\frac{5}{2} \varepsilon \varphi - \lambda \nabla T_e \right), \quad \vec{j} = q\vec{\phi}_e$$

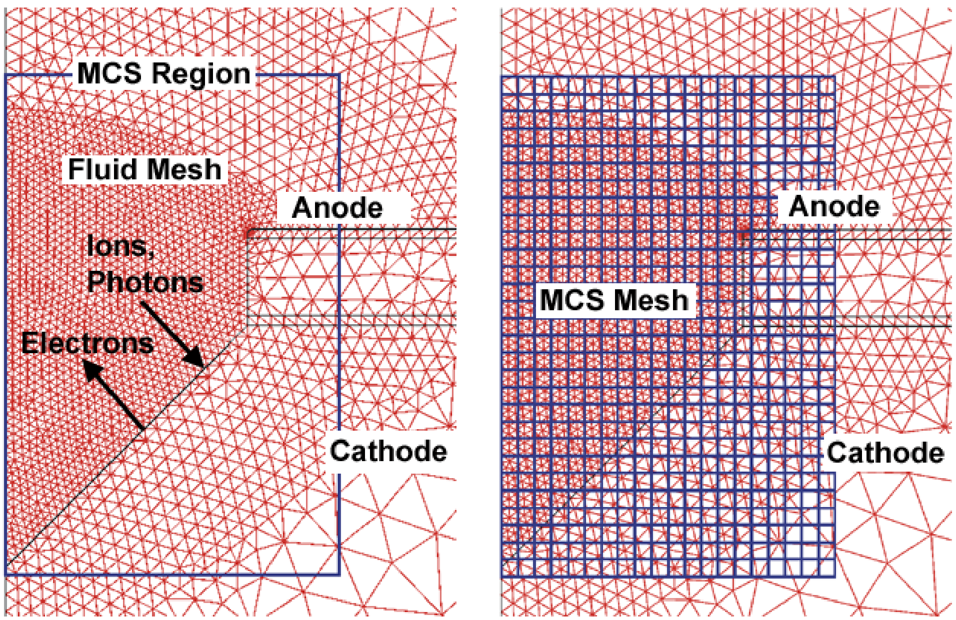
- **Neutral continuity and energy transport.**

$$\frac{\partial N_i}{\partial t} = -\nabla \cdot \left(\vec{v} - DN_o \nabla \left(\frac{N_i}{N_o} \right) \right) + S_i, \quad \frac{\partial (\rho c T)}{\partial t} = -\nabla \cdot \kappa \nabla T + P_g$$

University of Illinois
Optical and Discharge Physics

DESCRIPTION OF MODEL: MCS MESHING

- **Transport of energetic secondary electrons is addressed with a Monte Carlo Simulation.**

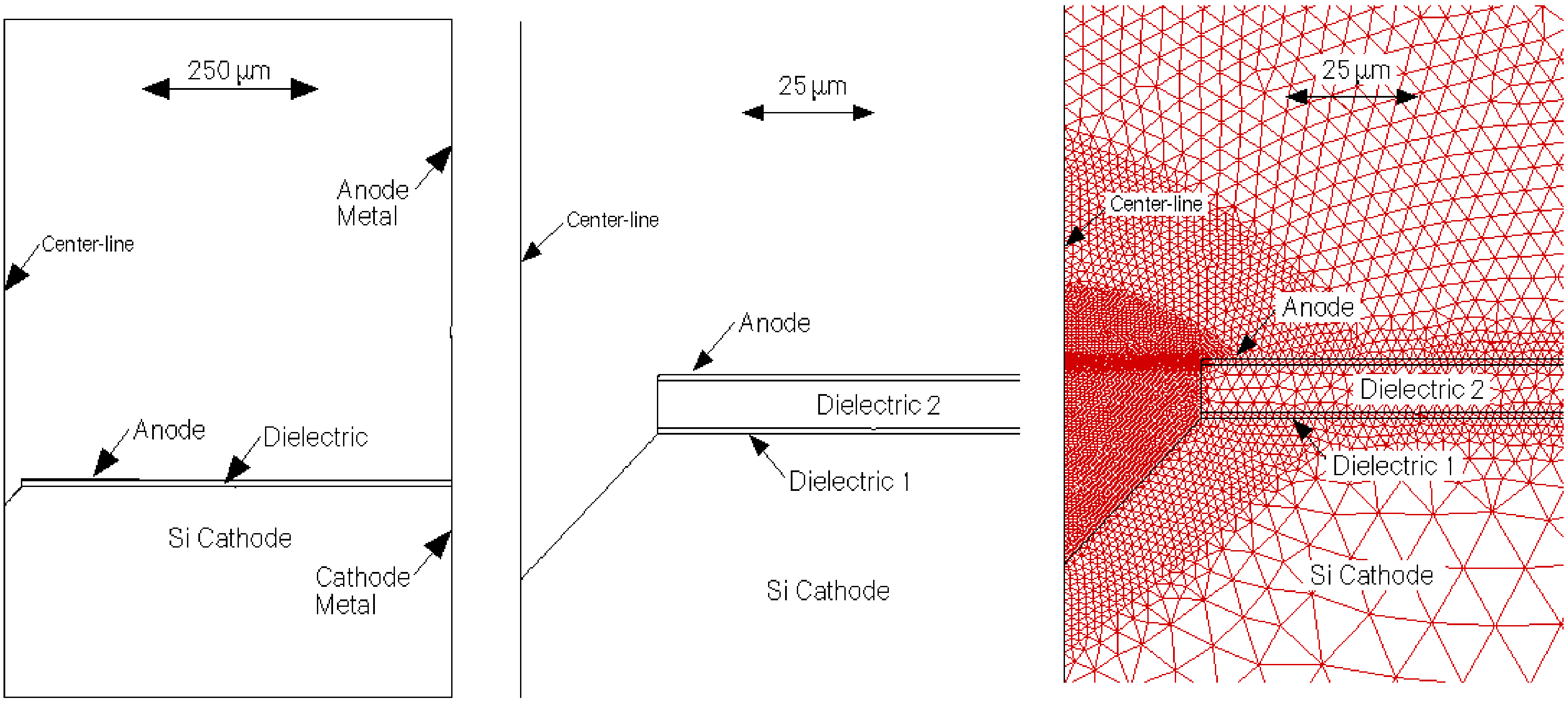


- **Superimpose Cartesian MCS mesh on unstructured fluid mesh. Construct Greens functions for interpolation between meshes.**
- **Electrons and their progeny are followed until slowing into bulk plasma or leaving MCS volume.**
- **Electron energy distribution is computed on MCS mesh.**
- **EED produces source functions for electron impact processes which are interpolated to fluid mesh.**

University of Illinois
Optical and Discharge Physics

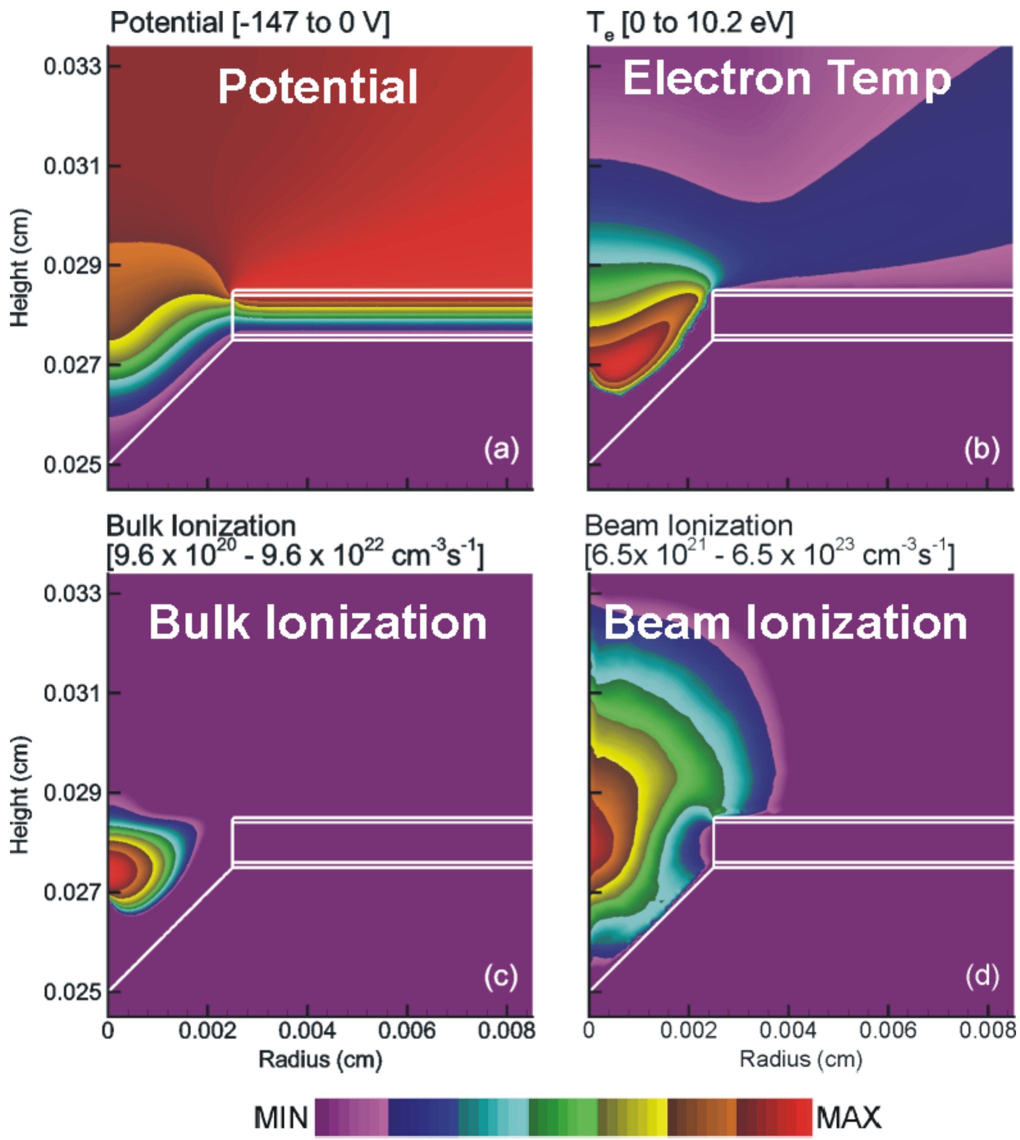
MODEL GEOMETRY: Si PYRAMID MICRODISCHARGE

- **Investigations of a cylindrically symmetric Si pyramid MD. Typical meshes have 5,000-10^4 nodes, dynamic range of 50-100.**



University of Illinois
Optical and Discharge Physics

BASE CASE: Ne, 600 Torr, 50 μm DIAMETER

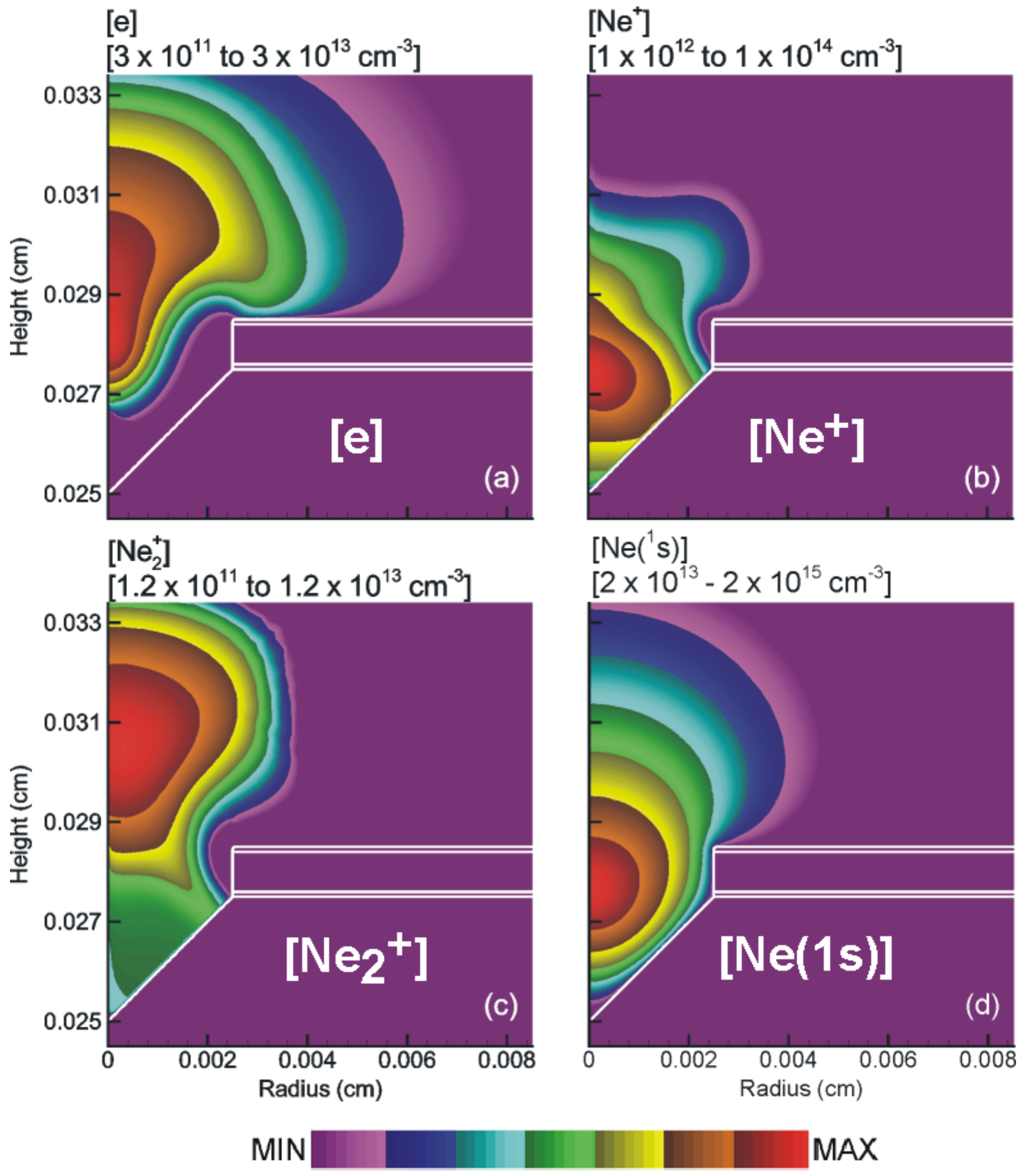


- **Optimum conditions produces large enough charge density to warp electric potential into cathode well.**
- **In spite of large Te, ionization is dominated by beam electrons.**

- **Ne, 600 Torr, 50 μm diameter, 200 V, 1 MΩ**

University of Illinois
Optical and Discharge Physics

BASE CASE: CHARGED PARTICLE DENSITIES

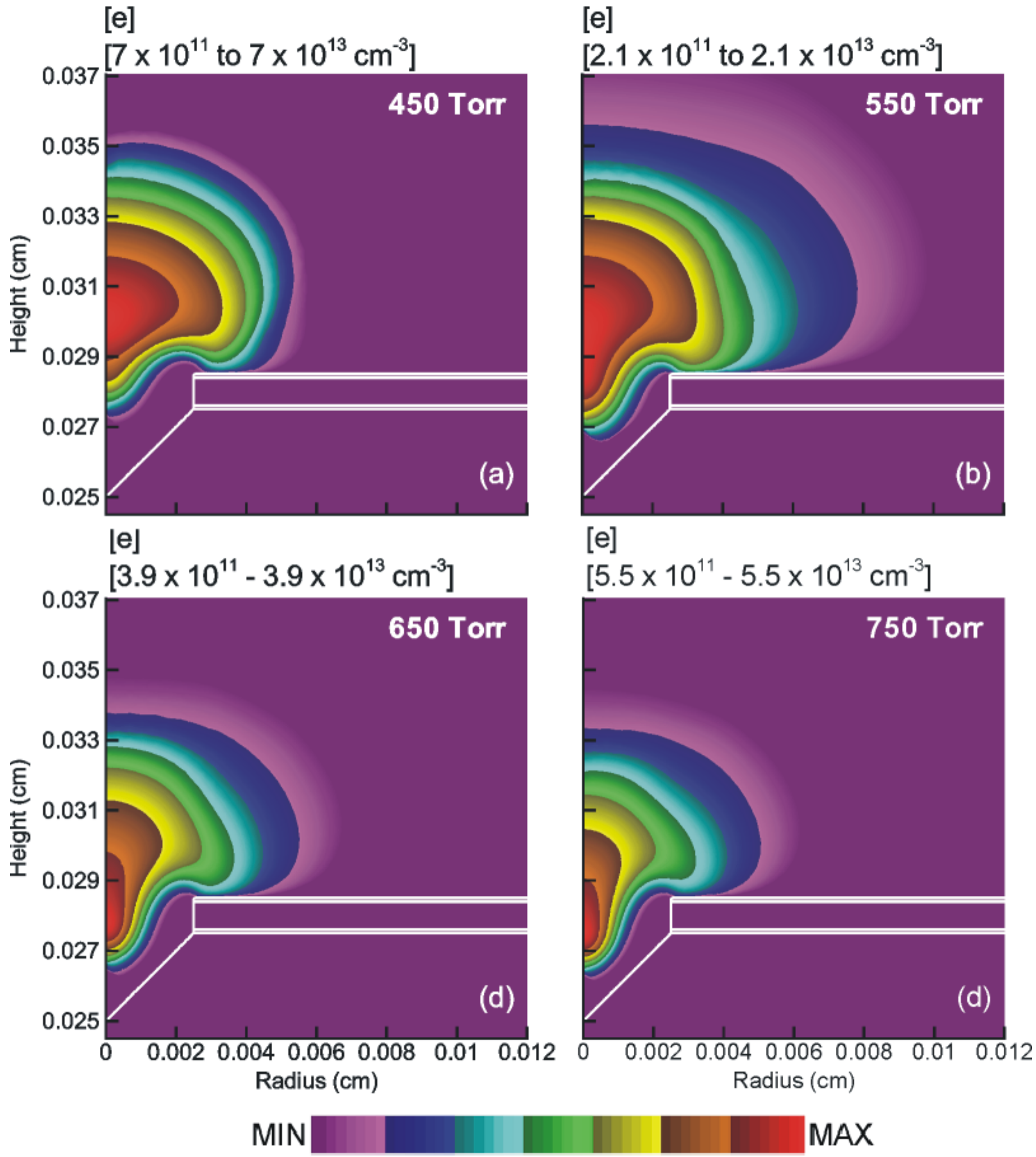


- Ne, 600 Torr, 50 μm diameter, 200 V, 1 MΩ

- There are few regions of quasi-neutrality or which are positive column-like.
- [e] > 10^{13} cm^{-3} for 10s μA.
- Excited state densities >10^{15} cm^{-3} are commensurate with macroscopic pulsed discharge devices.

University of Illinois
Optical and Discharge Physics

ELECTRON DENSITY vs PRESSURE

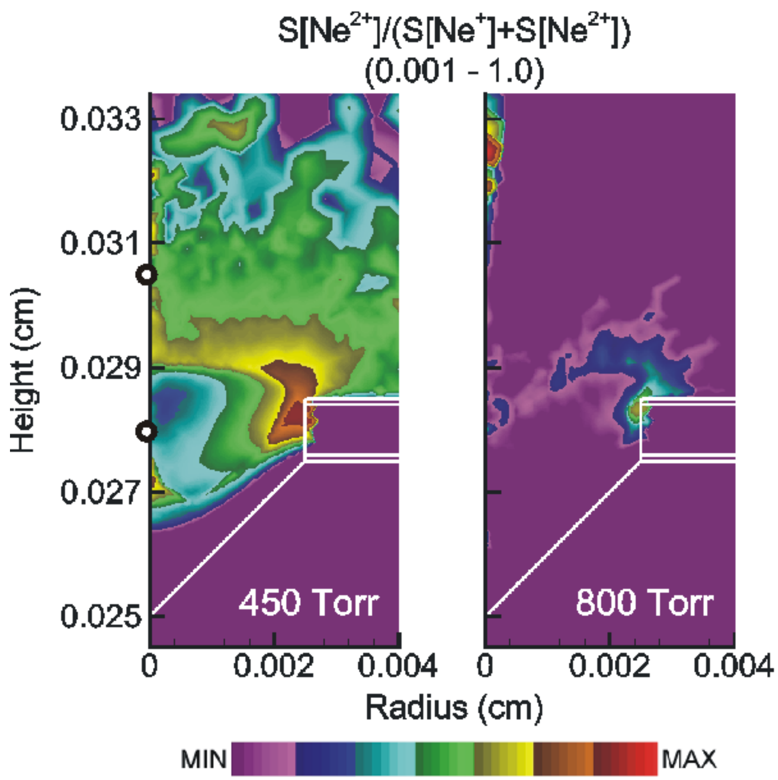


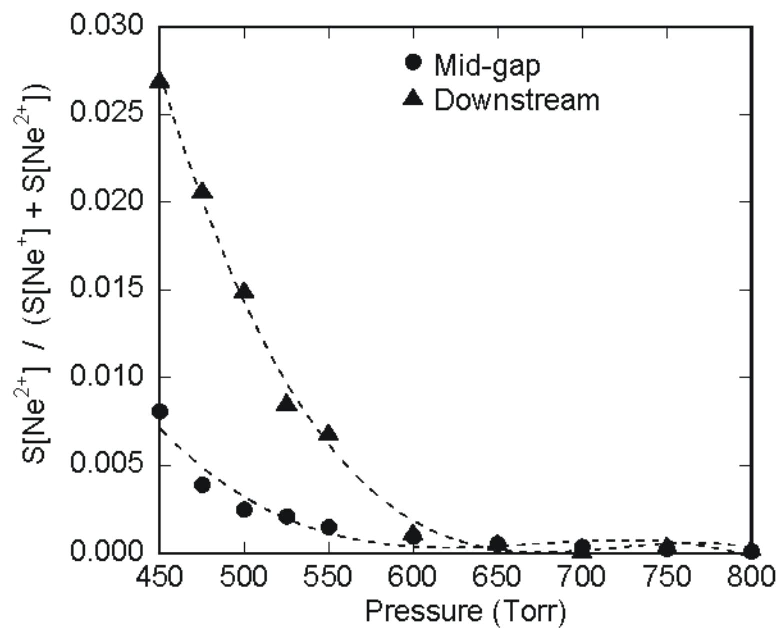
- **The discharge becomes more confined at higher pressures due to shorter stopping length of beam electrons.**

- **Ne, 50 μm diameter, 200-240 V, 1 MΩ**

BEAM vs BULK: NONEQUILIBRIUM IONIZATION SOURCES

- The threshold for Ne $\rightarrow$ Ne^{++} is 41 eV. Monitoring $S[Ne^{++}]/S[Ne^{+}]$ signals MD transitions from Townsend-like to negative glow-like.
- Negative glow-like excitation occurs with P < 550 Torr.

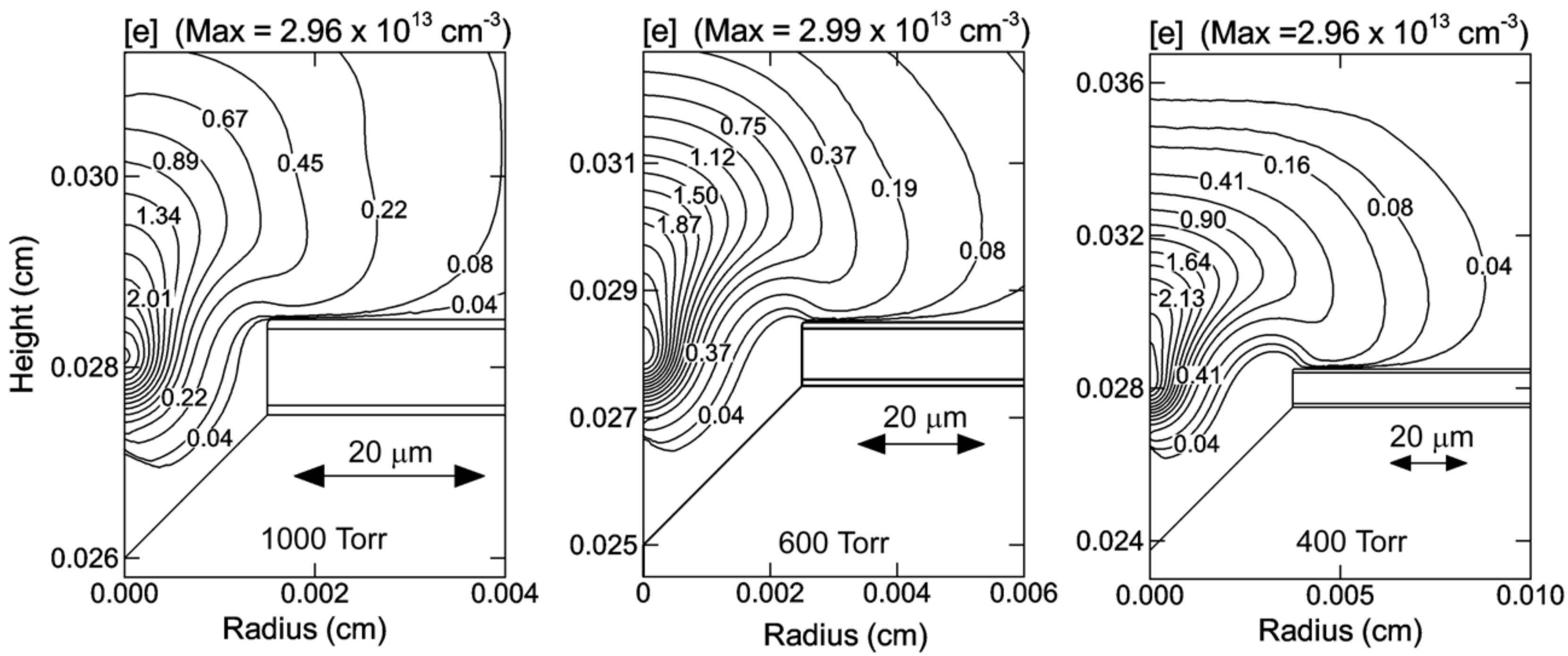




- Ne, 50 μm diameter, 200-240 V, 1 MΩ

SCALING WITH SIZE: pd, j = CONSTANT

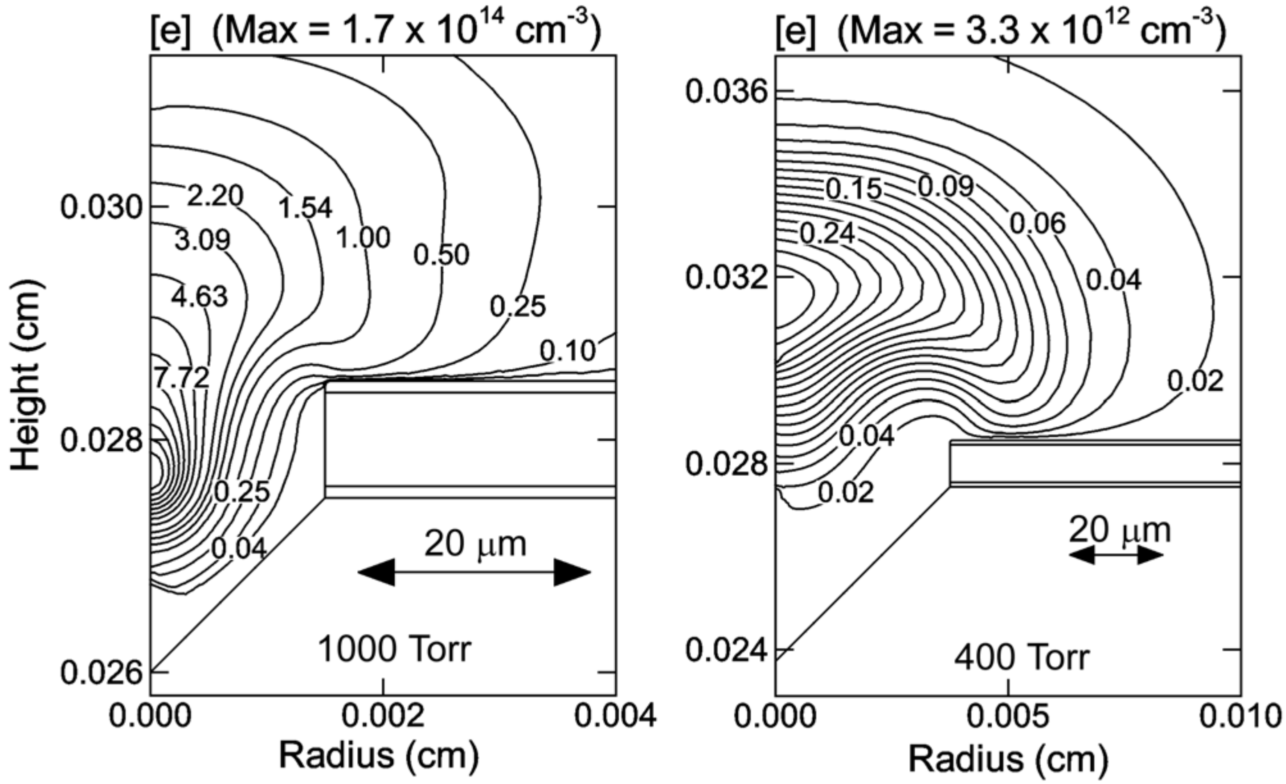
- Pd scaling should not be a steadfast expectation.
- Sheath properties scale with absolute plasma density and not pd.
- Scaling requires careful ballasting to keep [e] and sheath



- Ne, 200 V, 1 MΩ

SCALING WITH SIZE: pd, ballast = CONSTANT

- When keeping ballast constant, j decreases in larger devices, resulting in lower electron density, less shielding, more “electrostatic” equilibrium. Electron cloud “pops” out of cavity.



- Ne, 200 V, 1 MΩ

CONCLUDING REMARKS and ACKNOWLEDGEMENTS

- Nonequilibrium in plasma processing is everywhere you look…
  - Electromagnetics
  - Plasma dynamics
  - Surface chemistry
  - Electrostatics
- The development of computational and experimental techniques to resolve non-equilibrium will continue to be important in improving our fundamental understanding of these processes.
- Collaborators
  - Dr. Alex Vasenkov
  - Mr. Arvind Sankaran