

MODELING OF MICRODISCHARGE DEVICES: PLASMA AND GAS DYNAMICS*

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AGENDA

- **Scaling of Microdischarge Devices**
- **Description of model**
- **The annular sandwich MD**
- **The pyramidal MD**
- **Concluding Remarks.**

- **Acknowledgements: Ramesh Arakoni, Ananth Bhoj, Brian Lay**

MICRODISCHARGE PLASMA SOURCES

- Microdischarges have demonstrated great promise for photon, radical and ionization sources, and laboratories for plasma and optical physics.
- Microdischarges leverage pd scaling to operate as dc atmospheric glows 10s –100s μm in size.
- MEMS 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.

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

$$L_{\text{cathodeFall}} = (2V_c \epsilon_0 / (qn_I))^{1/2} \approx 10 - 20 \mu\text{m}$$

WHAT CAN BE LEARNED FROM MODELING MICRODISCHARGES?

- **Progress in other fields of low temperature plasmas has greatly benefited and been facilitated by modeling.**
 - **Plasma materials processing**
 - **Lasers**
 - **Pollution abatement**
- **Development of microdischarge technologies has been extremely successful without a strong legacy of modeling.**
- **What can be learned from modeling microdischarges (that we didn't already know)?**
- **What capabilities in modeling are required?**

GOAL FOR THIS TALK: MODELING AS A BASIS OF FUNDAMENTAL UNDERSTANDING AND SCALING

- Discussion of modeling MDs with goals of
 - Fundamental parameters and operating characteristics
 - Scaling
 - Use of MDs as sources of radicals and thrust
- Modeling Platform: *Nonpdpsim* 2-dimensional plasma hydrodynamics model

DESCRIPTION OF nonPDPSIM

- To investigate scaling processes in microdischarge sources, nonPDPSIM has been developed, a 2-dimensional model.
 - Rectilinear or cylindrical unstructured mesh
 - Implicit drift-diffusion-advection for charged species
 - Navier-Stokes for neutral species
 - Poisson's equation (volume, surface charge, material conduction.
 - Circuit model
 - Electron energy equation coupled with Boltzmann solution
 - Monte Carlo beam electrons
 - Optically thick radiation transport with photoionization
 - Secondary electrons by impact, thermionics, photo-emission
 - Surface chemistry.

DESCRIPTION OF MODEL: CHARGED PARTICLE, SOURCES

- **Continuity (sources from electron and heavy particle collisions, surface chemistry, photo-ionization, secondary emission), fluxes by modified Sharfetter-Gummel with advective flow field.**

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

- **Poisson's Equation for Electric Potential: $-\nabla \cdot \epsilon \nabla \Phi = \rho_V + \rho_S$**
- **Photoionization, electric field and secondary emission:**

$$S_{Pi}(\vec{r}) = \int \frac{N_i(\vec{r}) \sigma_{ij} N_j(\vec{r}') \exp\left(\frac{-|\vec{r}' - \vec{r}|}{\lambda}\right) d^3 \vec{r}'}{4\pi |\vec{r}' - \vec{r}|^2}$$

$$S_{Si} = -\nabla \cdot \mathbf{j}, \quad j_E = AT^2 \exp\left(\frac{-\left(\Phi_w - (q^3 E / \epsilon_0)^{1/2}\right)}{kT_s}\right), \quad j_S = \sum_j \gamma_{ij} \phi_j$$

DESCRIPTION OF MODEL: ELECTRON ENERGY, TRANSPORT COEFFICIENTS

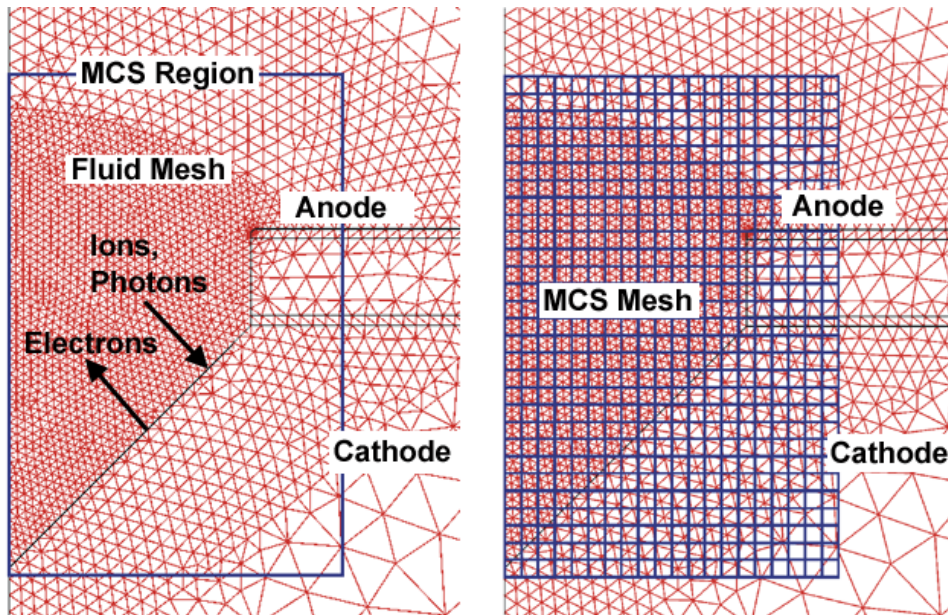
- Electron energy equation implicitly integrated using Successive-Over-Relaxation:

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

- Electron transport coefficients obtained from 2-term spherical harmonic expansion of Boltzmann's Equation.
- Ion transport coefficients obtained from tabulated values from the literature or using conventional approximation techniques.

DESCRIPTION OF MODEL: MCS AND 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.

DESCRIPTION OF MODEL: NEUTRAL PARTICLE TRANSPORT

- Fluid averaged values of mass density, mass momentum and thermal energy density obtained using unsteady, compressible algorithms.

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \vec{v}) + (\text{inlets, pumps})$$

$$\frac{\partial(\rho \vec{v})}{\partial t} = \nabla(NkT) - \nabla \cdot (\rho \vec{v} \vec{v}) - \nabla \cdot \bar{\mu} + \sum_i q_i N_i \vec{E}_i$$

$$\frac{\partial(\rho c_p T)}{\partial t} = -\nabla(-\kappa \nabla T + \rho \vec{v} c_p T) + P_i \nabla \cdot \mathbf{v}_f - \sum_i R_i \Delta H_i + \sum_i \vec{j}_i \cdot \vec{E}$$

- Alternately, if only heat conduction is considered.

$$\frac{\partial(\rho c_p T)}{\partial t} = -\nabla(-\kappa \nabla T) - \sum_i R_i \Delta H_i + \sum_i \vec{j}_i \cdot \vec{E}$$

DESCRIPTION OF MODEL: NEUTRAL PARTICLE UPDATE

- Transport equations are implicitly solved using **Successive-Over-Relaxation**:

$$N_i(t + \Delta t) = N_i(t) - \nabla \cdot \left(\vec{v}_f - D_i N_T \nabla \left(\frac{N_i(t + \Delta t)}{N_T} \right) \right) + S_V + S_S$$

- Surface chemistry is addressed using “flux-in/flux-out” boundary conditions with reactive sticking coefficients

$$S_{Si} = \sum_j (\nabla \cdot \vec{\phi}_j) \gamma_{ij}$$

METHOD OF SOLUTION

- **Finite volume techniques are used for flux conservation at all nodes.**

$$\frac{dN_i}{dt} = -\nabla \cdot \vec{\phi}_i = \frac{1}{V_i} \sum_j A_{ij} \phi_{ij}, \quad \phi_{ij} = \frac{1}{2} (\vec{\phi}_i + \vec{\phi}_j) \cdot \hat{a}_{ij}$$

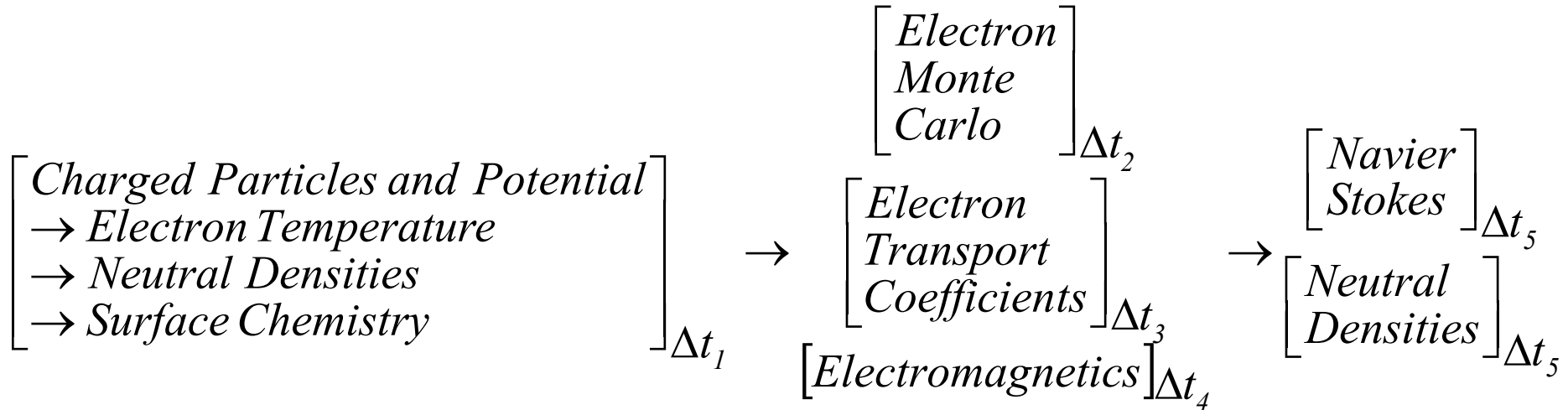
- **Jacobian elements are numerically derived to produce a matrix of differential updates for timestep Δt .**

$$N_i(t + \Delta t) = N_i(t) + \Delta N_i$$
$$\Delta N_i = \frac{\partial N_i}{\partial t}(t) \cdot \Delta t + \sum_j \left(\frac{\partial N_i}{\partial N_j} \right) \Delta N_j$$

- **Iterative Newton's method is used to solved coupled charged particle transport and Poisson's equation.**

METHOD OF SOLUTION

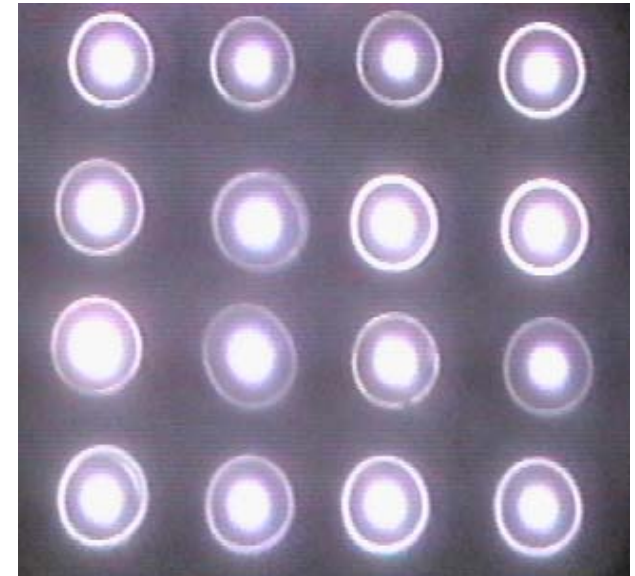
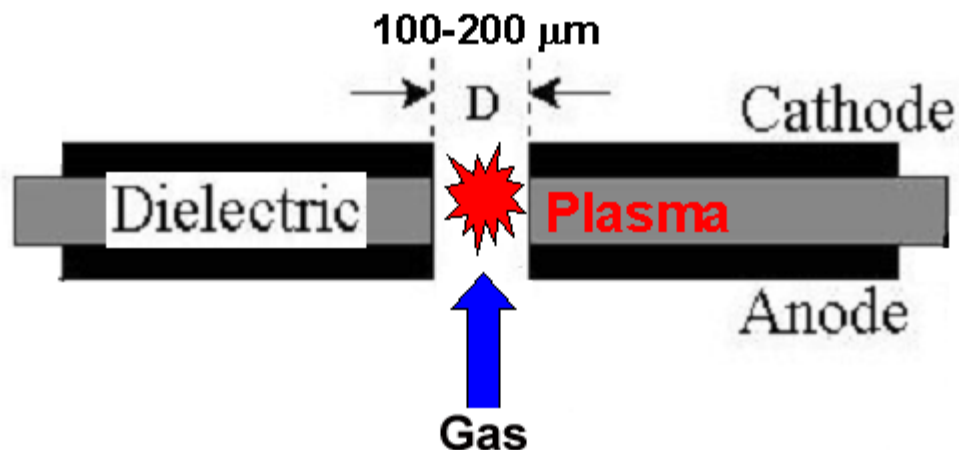
- Time splicing acceleration techniques are used in which modules are sequentially executed.



- If only the steady state is desired, the time steps taken in each module are usually different.

ANNULAR SANDWICH MICRODISCHARGE

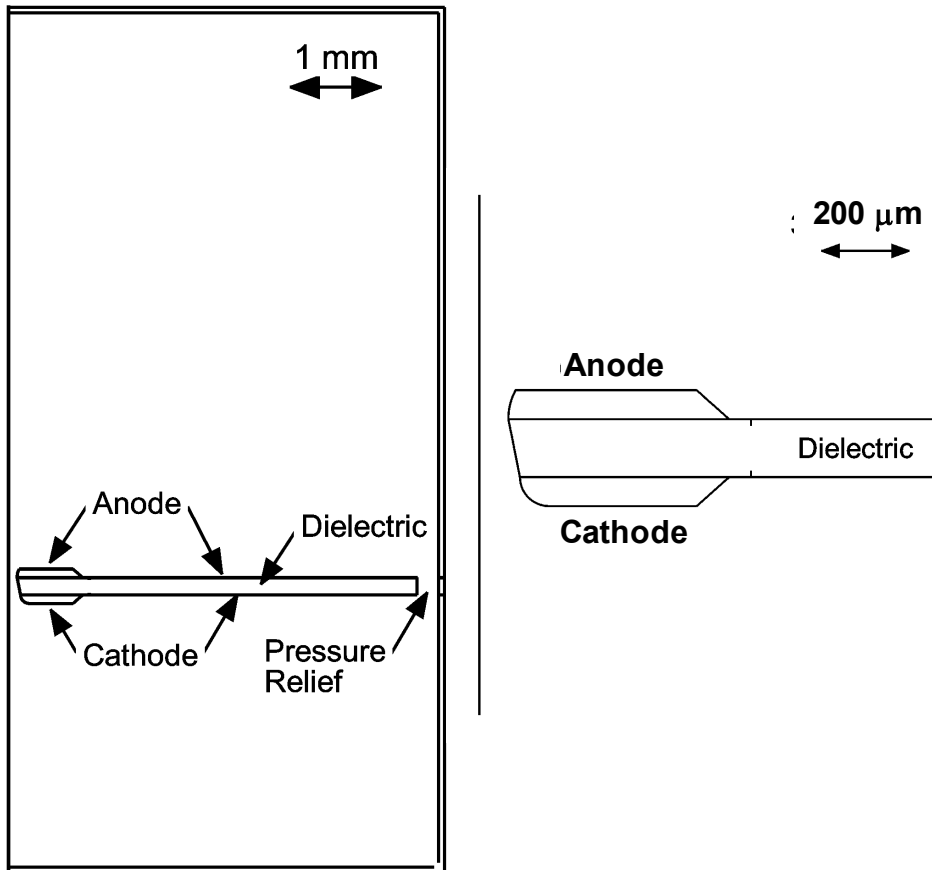
- MDs with 10s - 100s μm spacing with circular/annular electrode cavity.
- Operation of up to 1 atm in rare and molecular gases.
- 150-300 V, a few mA



- Ref: Kurt Becker, GEC 2003

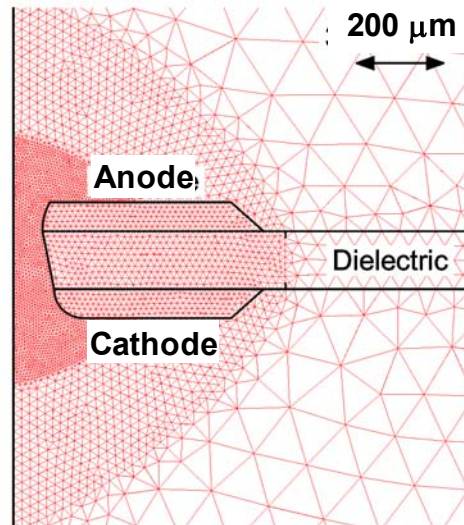
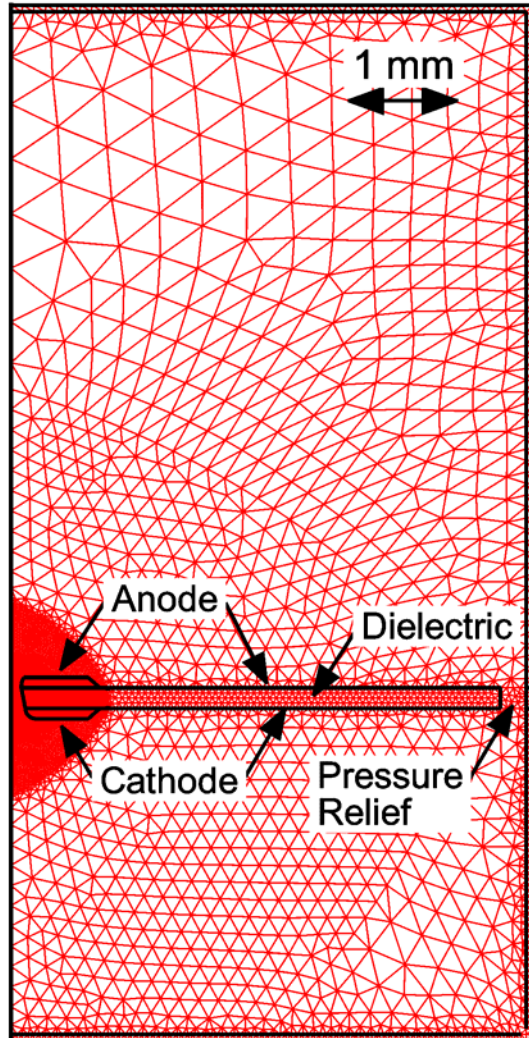
BASE CASE MICRODISCHARGE PARAMETERS

- A “sandwich” microdischarge device is the base case:



- Sloped dielectric (flow issues)
- Hole: 200 μm diameter at anode to 300 μm at cathode.
- Dielectric: 200 μm thick
- Anode/Cathode 100 μm thick
- Cylindrically symmetric
- Argon, 250 Torr, 2 mA (set by adjusting ballast resistor)

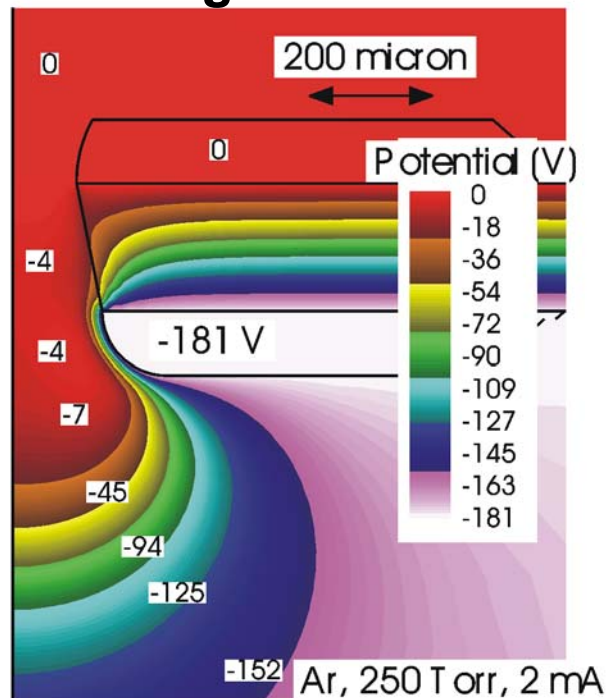
MESHING IS CRITICAL...



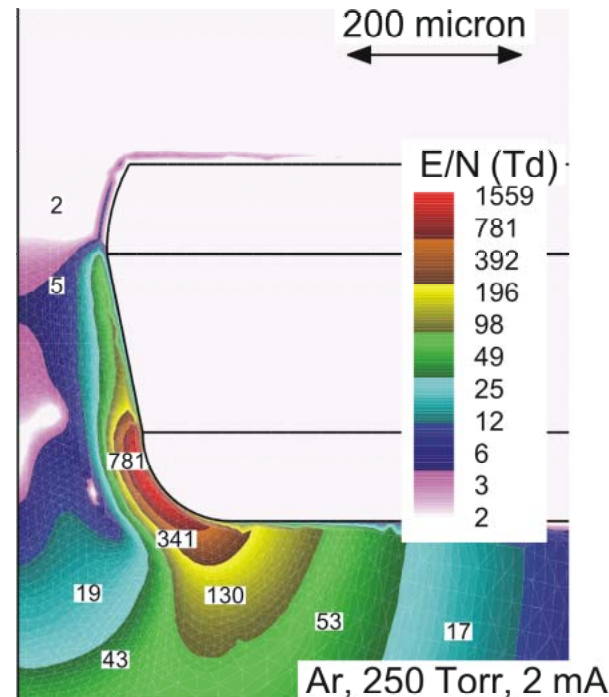
- The choice of meshing is critical in resolving plasma transport in the discharge zone.
- Must resolve cathode fall as well as electrical and flow boundary conditions at large distances.
- Dynamic range 100-1000
- Total nodes: 5424
Plasma nodes: 3693

ELECTRIC POTENTIAL AND FIELDS

- Anode potential penetrates into lower plenum, producing hollow-cathode-like structure.
- Geometrical enhancement and space charge produce fields approaching 100 kV/cm.



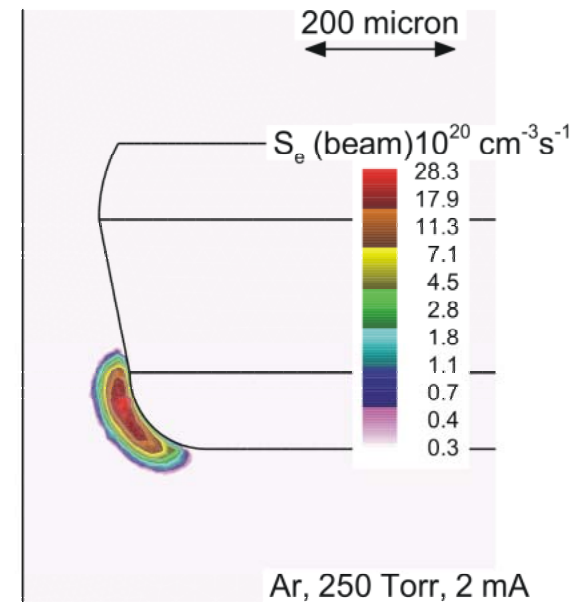
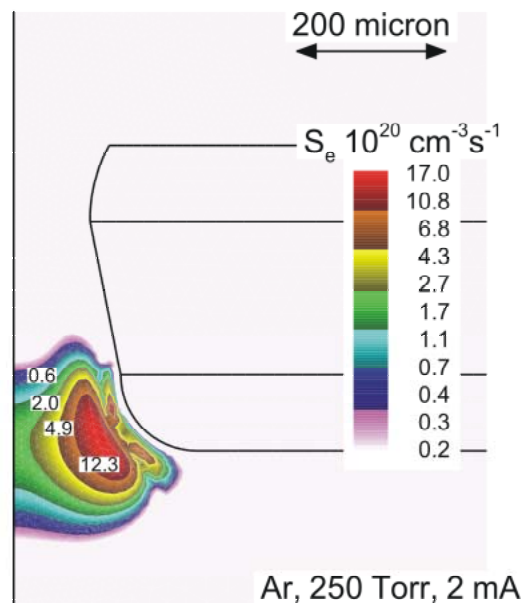
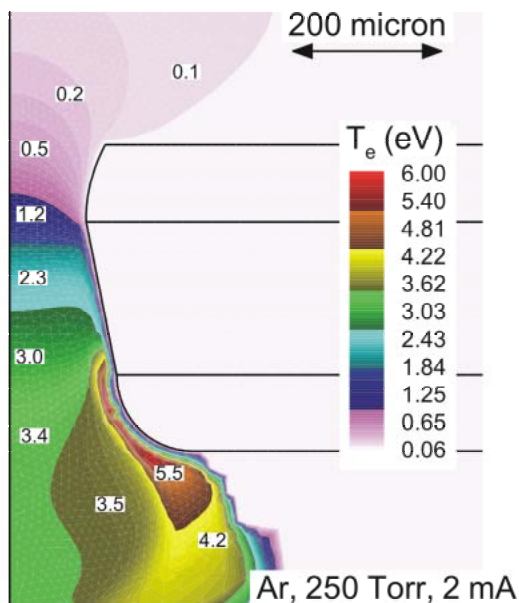
• Electric Potential



• E/N (Electric Field/Gas Density)
Max = 80 kV/cm

ELECTRON TEMPERATURE AND IONIZATION SOURCES

- In the bulk plasma, T_e of 3.5 eV suggests positive column conditions.
- Large contributions to ionization occur from both bulk and beam electrons



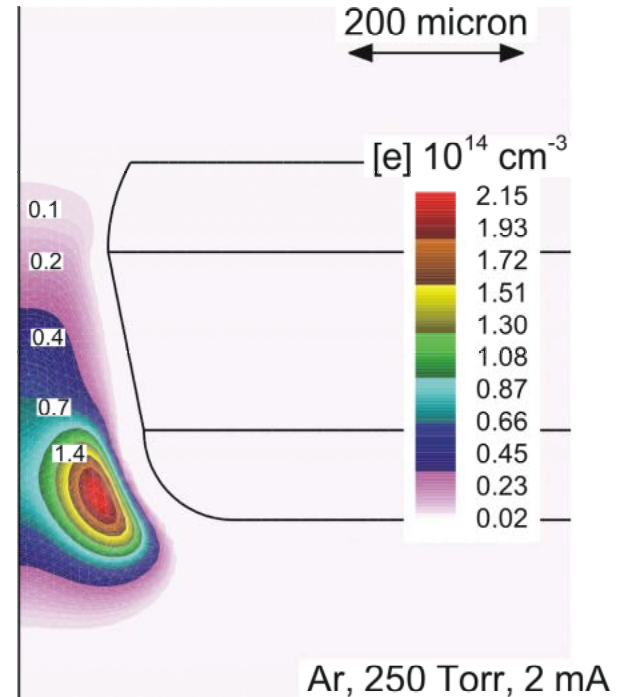
• Electron Temperature

• Bulk Ionization

• Beam ionization

ELECTRON DENSITY

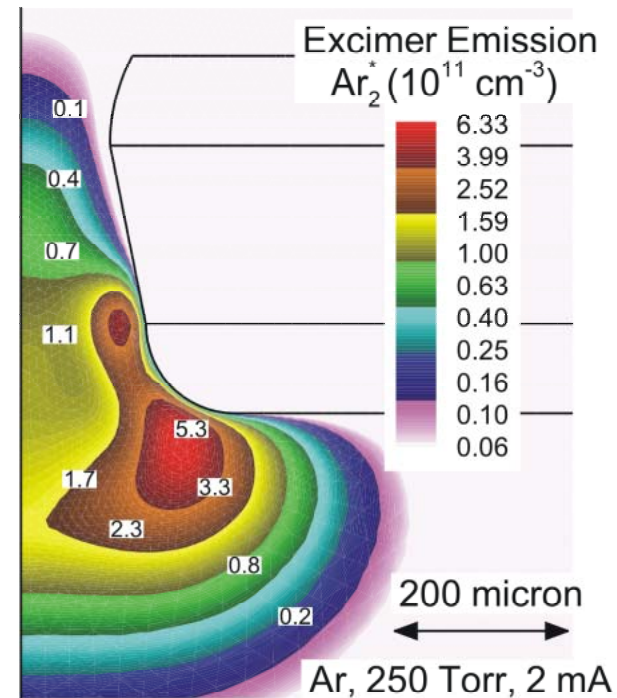
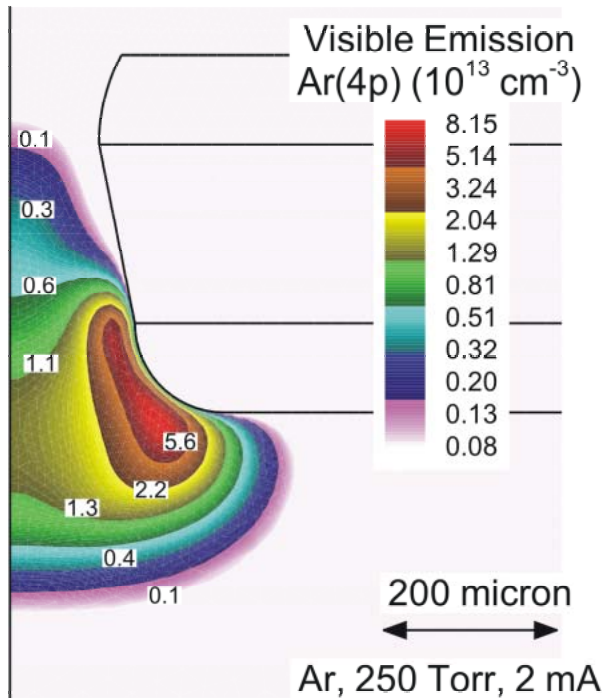
- Peak electron densities of $>10^{14} \text{ cm}^{-3}$ are produced in the steady state.
- These high cw densities enable large rates of excitation of high lying electronic states.



- Electron density

VISIBLE AND UV EMISSION

- **Visible emission is constrained to an annulus due to short lifetimes of states. UV emission from excimer is more distributed due to the large range of Ar(4s) metastable precursor.**

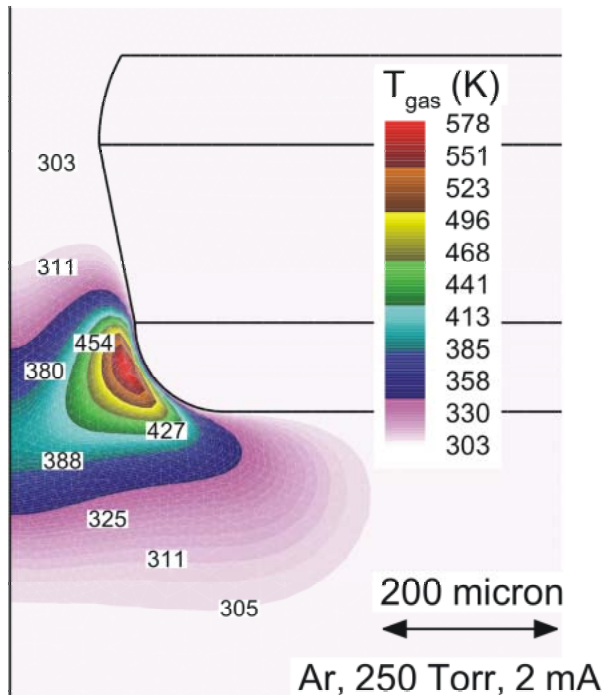


- **Ar(4p) Density (Visible Emission)**

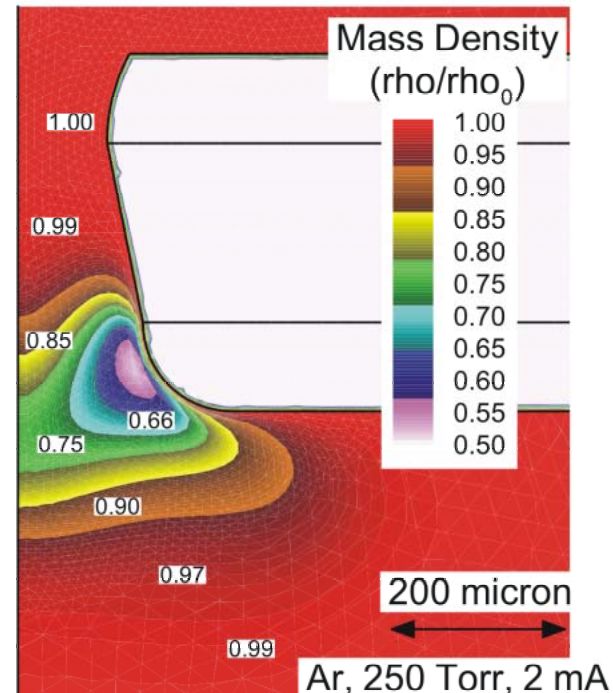
- **Ar₂* Density (UV Emission)**

THERMODYNAMIC PROPERTIES

- Current densities of 5-10 A/cm² and power of 10's-100 kW/cm³ produce significant gas heating and rarefaction.
- Rarefaction increases range of secondary electrons.



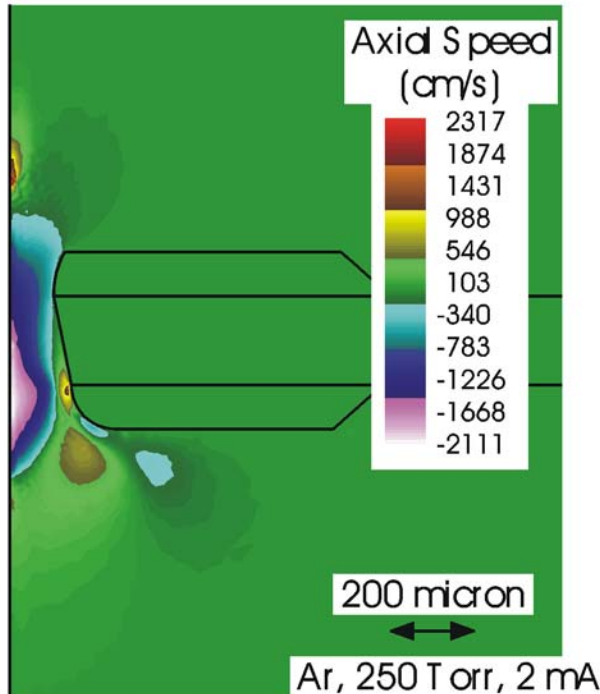
- Gas Temperature



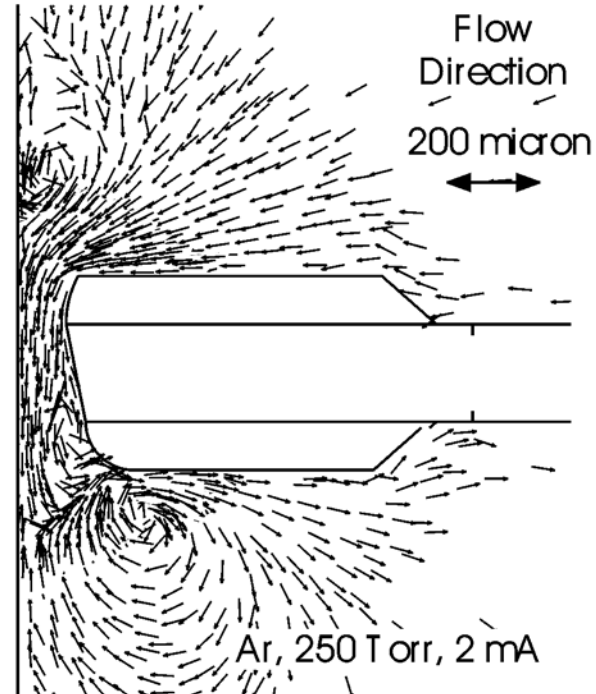
- Relative Mass Density

ADVECTIVE FLOWFIELD

- Cataphoresis entrains gas, producing pumping action from above the plenum, through the hole to below the plenum.
- The jet experiences resistance in the stagnation zone below the plenum and recirculation results.



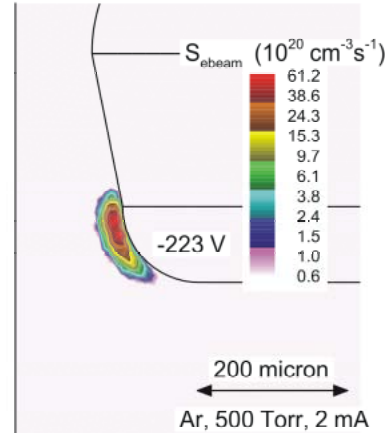
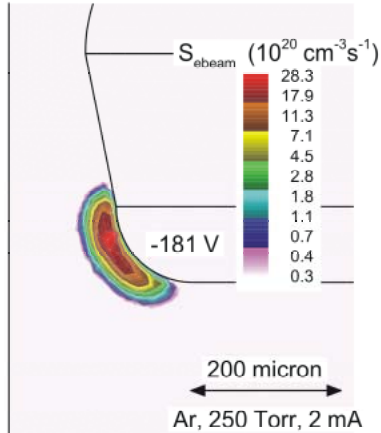
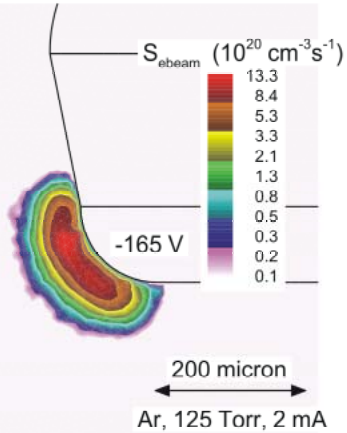
• Axial Gas Speed



• Flow Direction

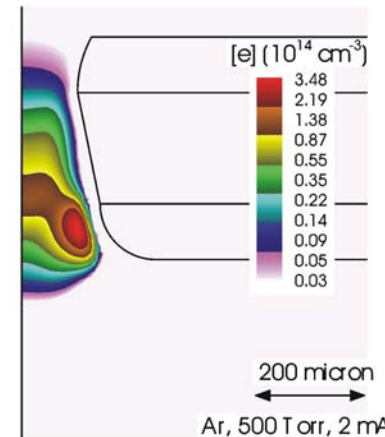
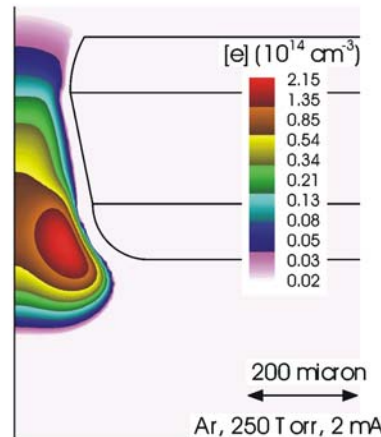
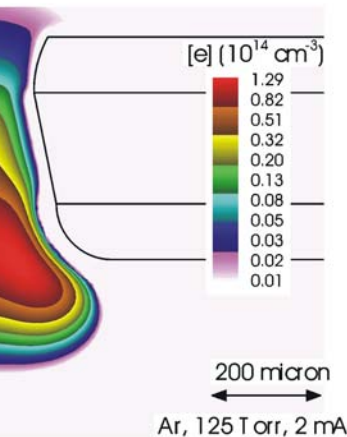
MD PROPERTIES vs PRESSURE

• Beam Ionization



- Decreasing pressure enables deeper penetration of beam electrons in spite of the lower cathode voltage.

• Electron Density



- The result is more confinement at higher pressure and higher peak electron density.
- Ar, 2 mA

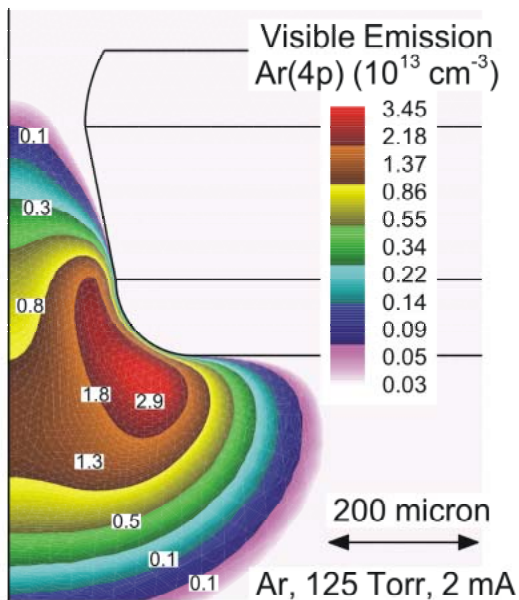
• 125 Torr
 1.3×10^{14}

• 250 Torr
 2.1×10^{14}

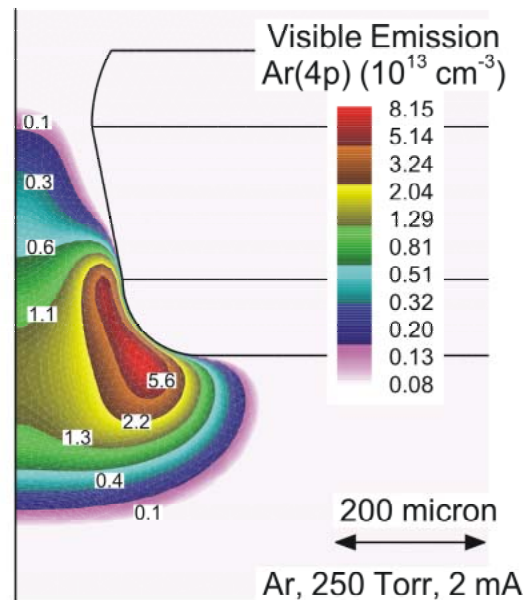
• 500 Torr
 3.5×10^{14}

MD PROPERTIES vs PRESSURE: VISIBLE EMISSION

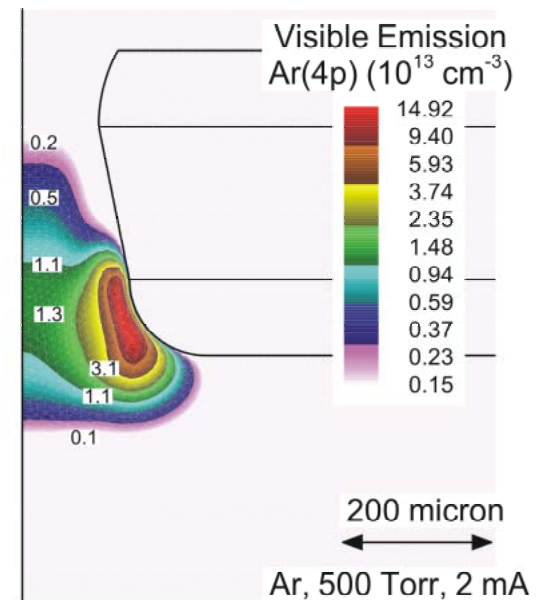
- Visible emission is significantly more extended at low pressure, penetrating far out the hole. Peak emission is greater at higher pressure due to confinement of beam component.



• 125 Torr

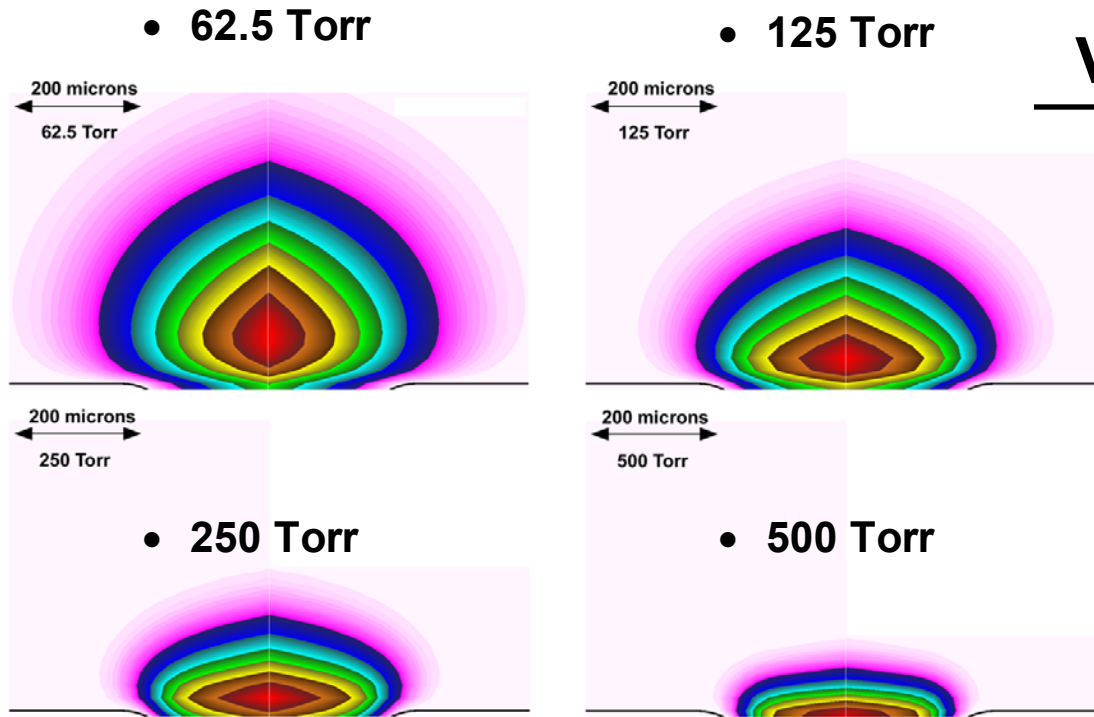


• 250 Torr

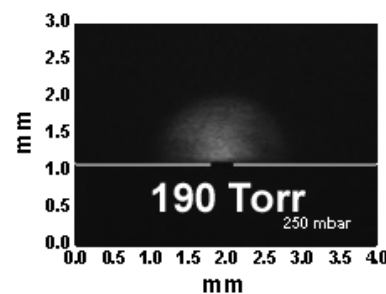
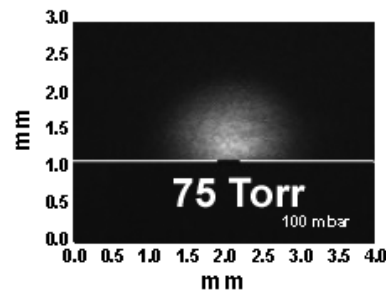
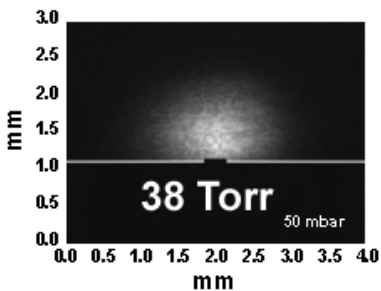


• 500 Torr

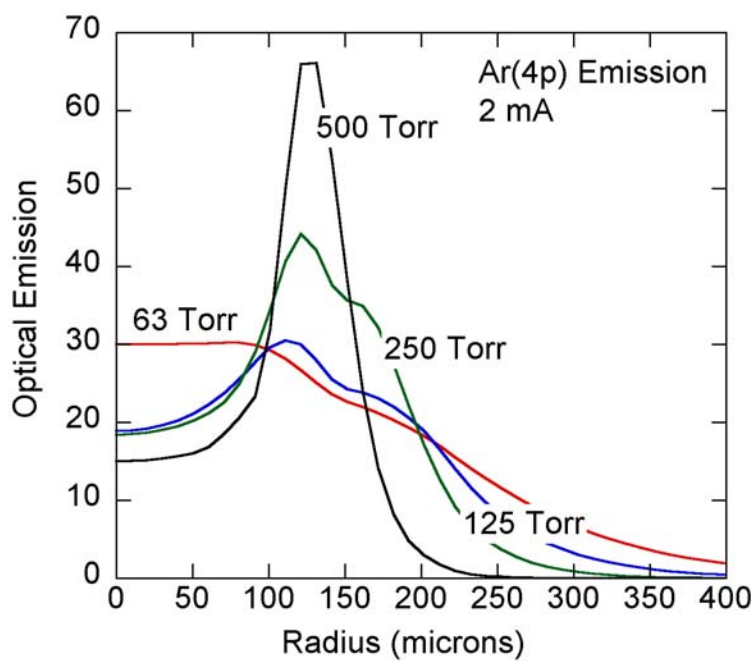
MD PROPERTIES vs PRESSURE: VISIBLE EMISSION



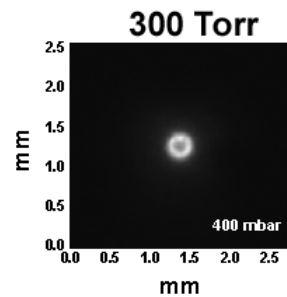
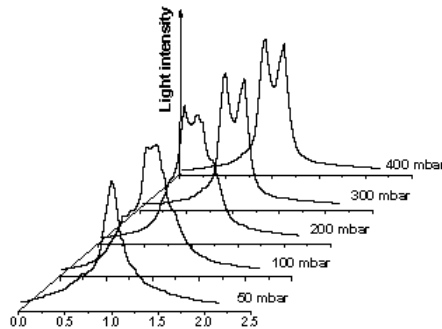
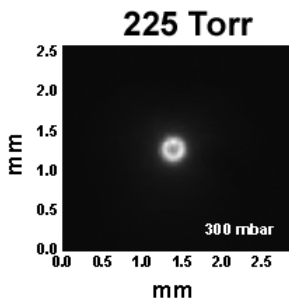
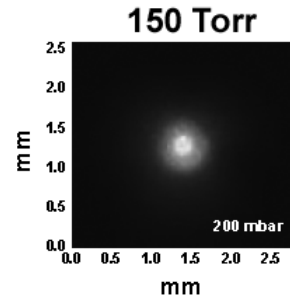
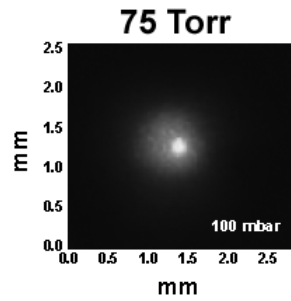
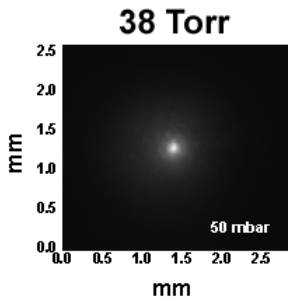
- Experimental trends are reproduced for contraction of optical emission at high pressure.
- Ref: Maria Cristina Penache, Thesis, 2002
- Ar, 2 mA, synthesized side views



MD PROPERTIES vs PRESSURE: VISIBLE EMISSION

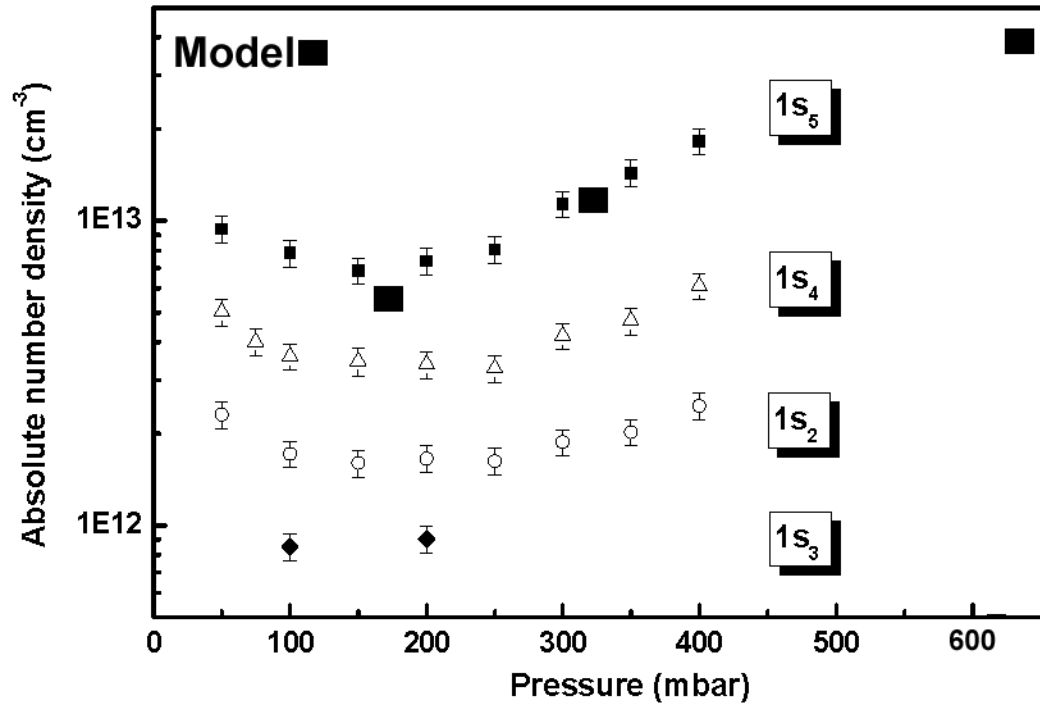


- Experimental trends are reproduced for contraction of optical emission with increasing pressure.
- Ref: Maria Cristina Penache, Thesis, 2002



MD PROPERTIES vs PRESSURE: Ar(4s) DENSITY

- Large metastable densities produce efficient excimer emission at higher pressures.

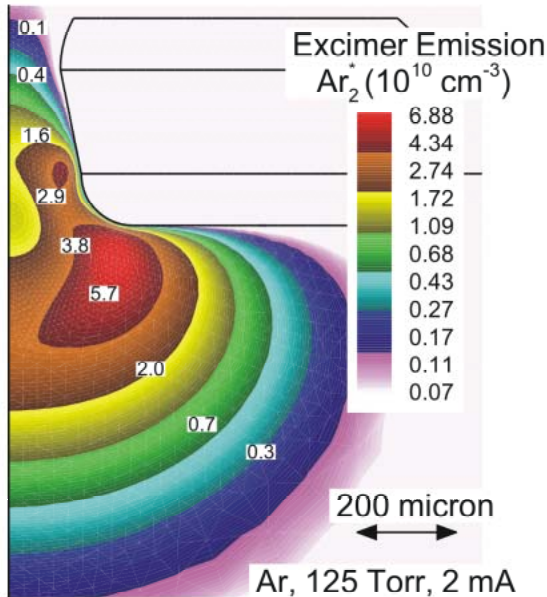


- Ref: Maria Cristina Penache, Thesis, 2002

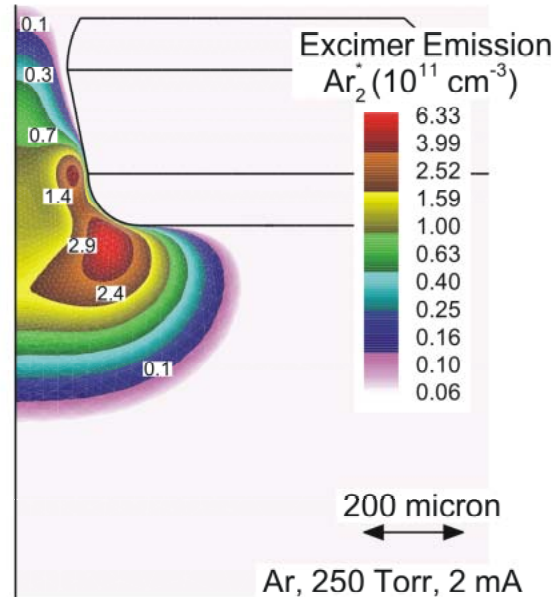
- Ar, 2 mA

MD PROPERTIES vs PRESSURE: UV-EXCIMER EMISSION

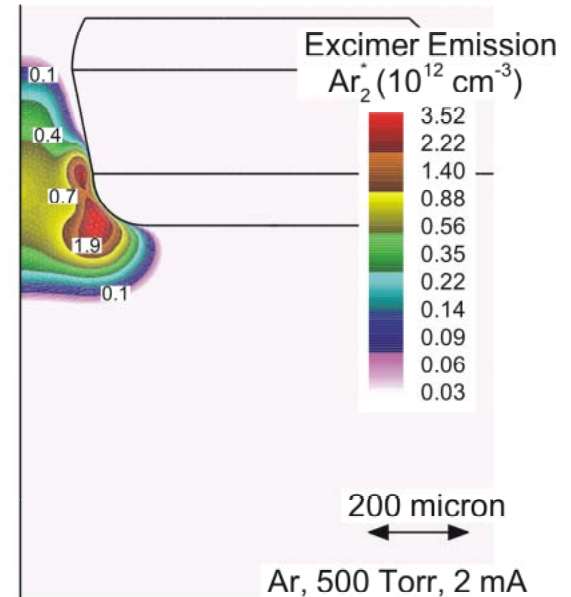
- The disparity between uniformity of and peak emission is greater for the UV-excimer due to greater diffusivity of Ar(4s) at low pressure and higher rate of dimer formation at high pressure.



• 125 Torr



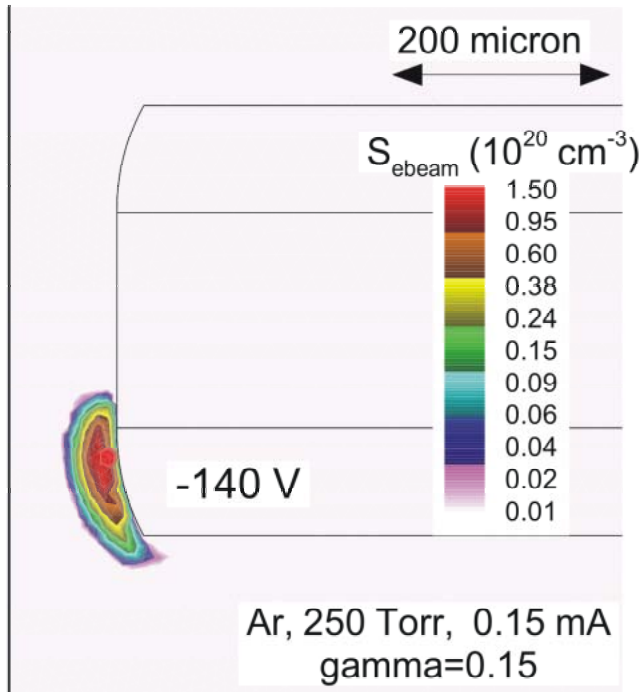
• 250 Torr



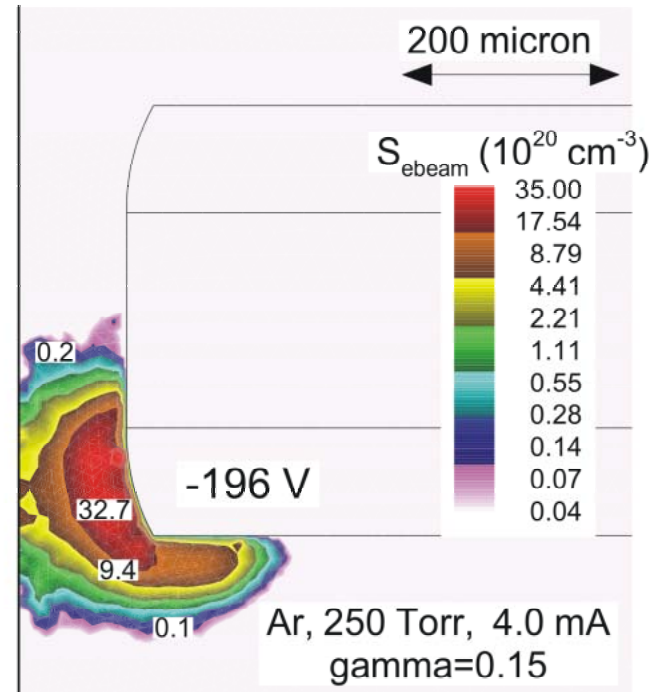
• 500 Torr

MD PROPERTIES vs CURRENT: BEAM IONIZATION

- Thermodynamics cannot be ignored in operation of MDs. Contrasting, low (0.15 mA) and high (4.0 mA) operation, the physical extent of beam ionization is greater at the higher current.



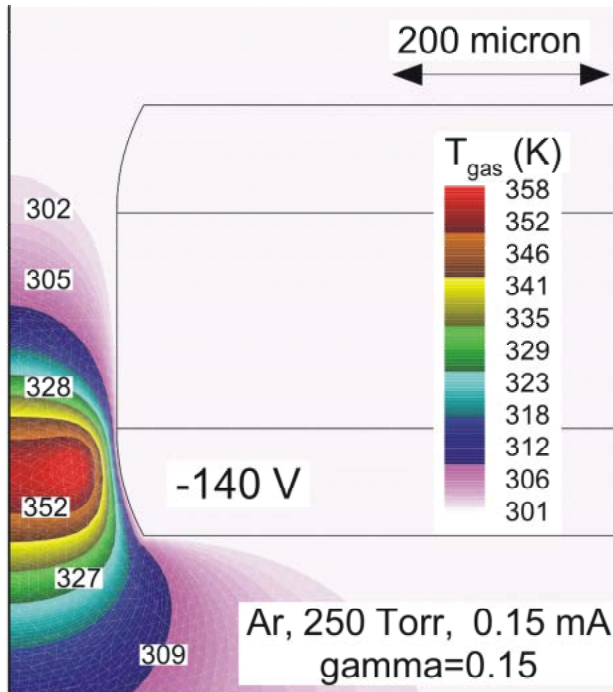
• 0.15 mA



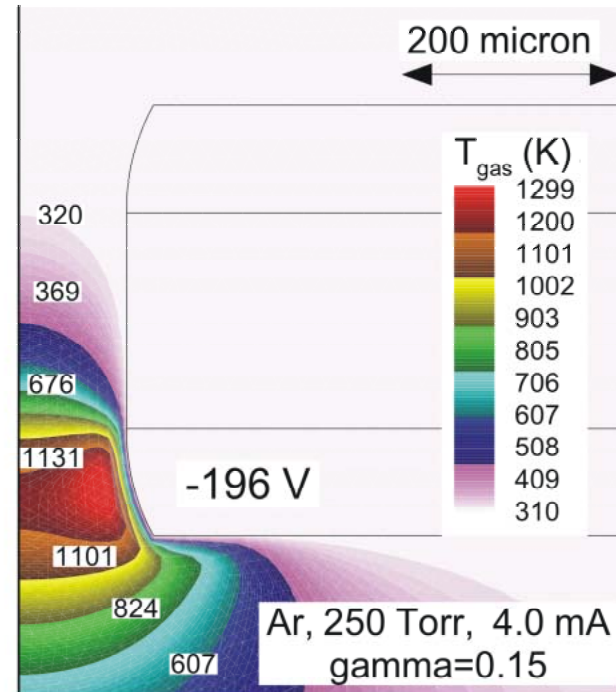
• 4.0 mA

MD PROPERTIES vs CURRENT: GAS TEMPERATURE

- ...which results in part from larger cathode voltage and in part from rarefaction produced by gas heating.



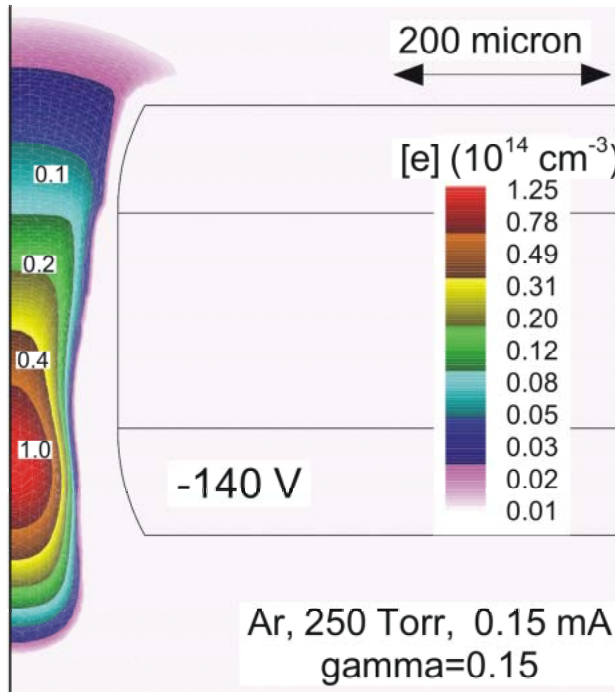
• 0.15 mA



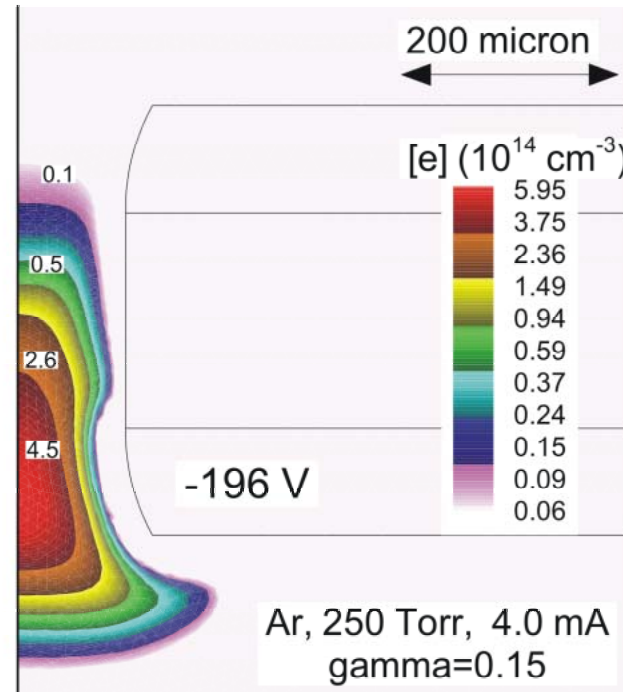
• 4.0 mA

MD PROPERTIES vs CURRENT: ELECTRON DENSITY

- The end result is a more tightly confined plasma at the lower pressure.



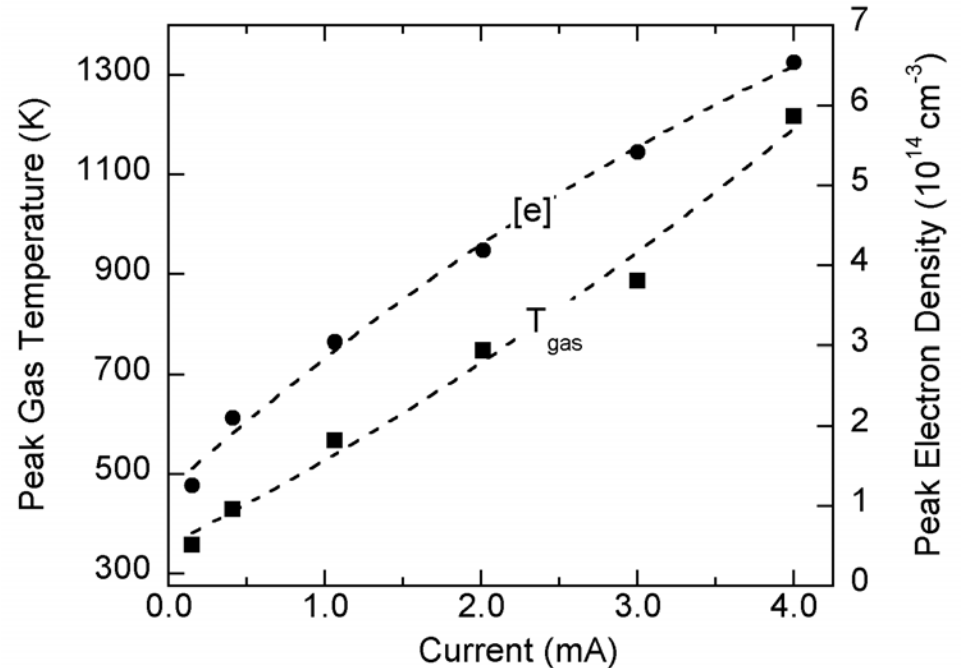
• 0.15 mA



• 4.0 mA

MD PROPERTIES vs CURRENT: T(gas), [e]

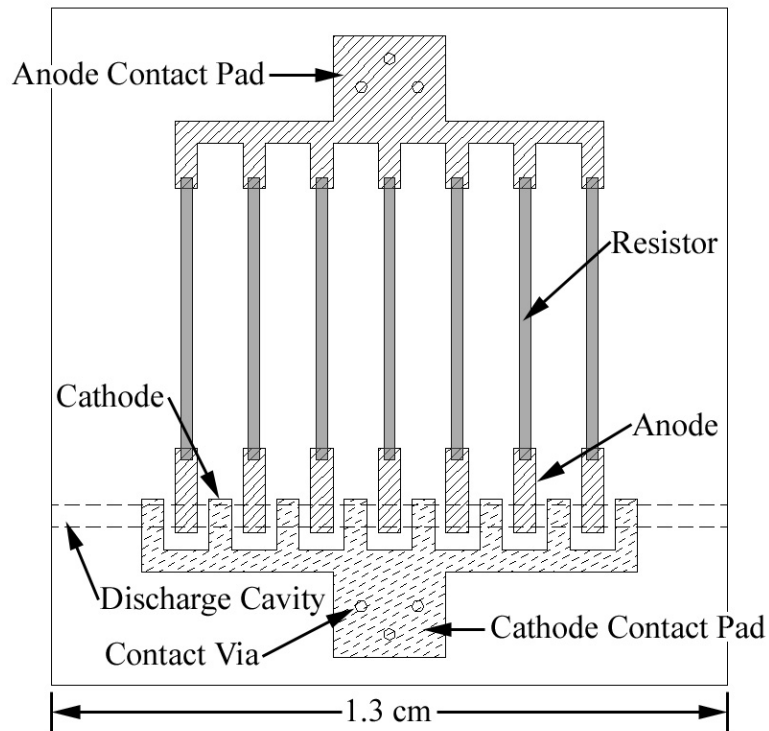
- Peak electron density and gas temperature scales nearly linearly with current density.



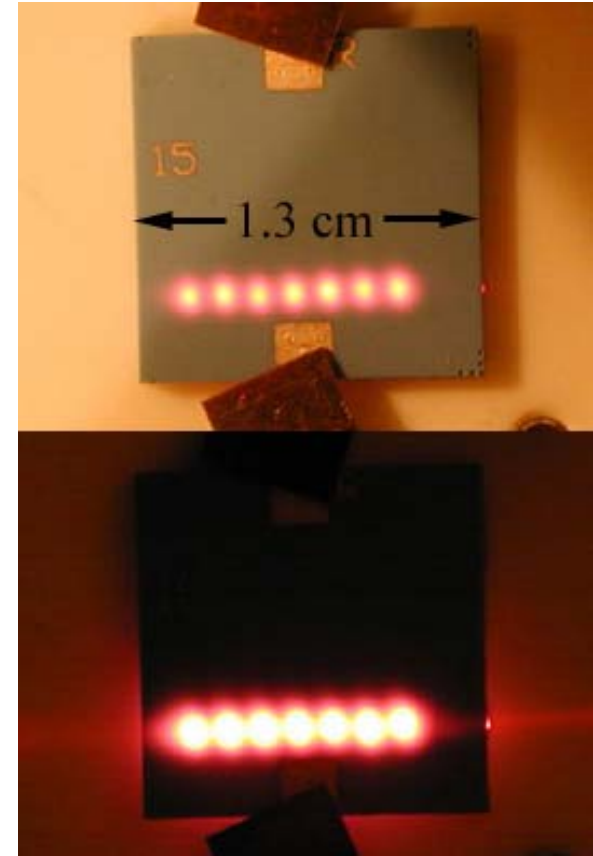
- Ar, 250 Torr, $\gamma = 0.15$

MULTISTAGE DEVICES

- Multistage MDs are desirable for long gain lengths for lasers.
- The design of such devices requires attention to thermodynamics issues.



• Ref: J. G. Eden

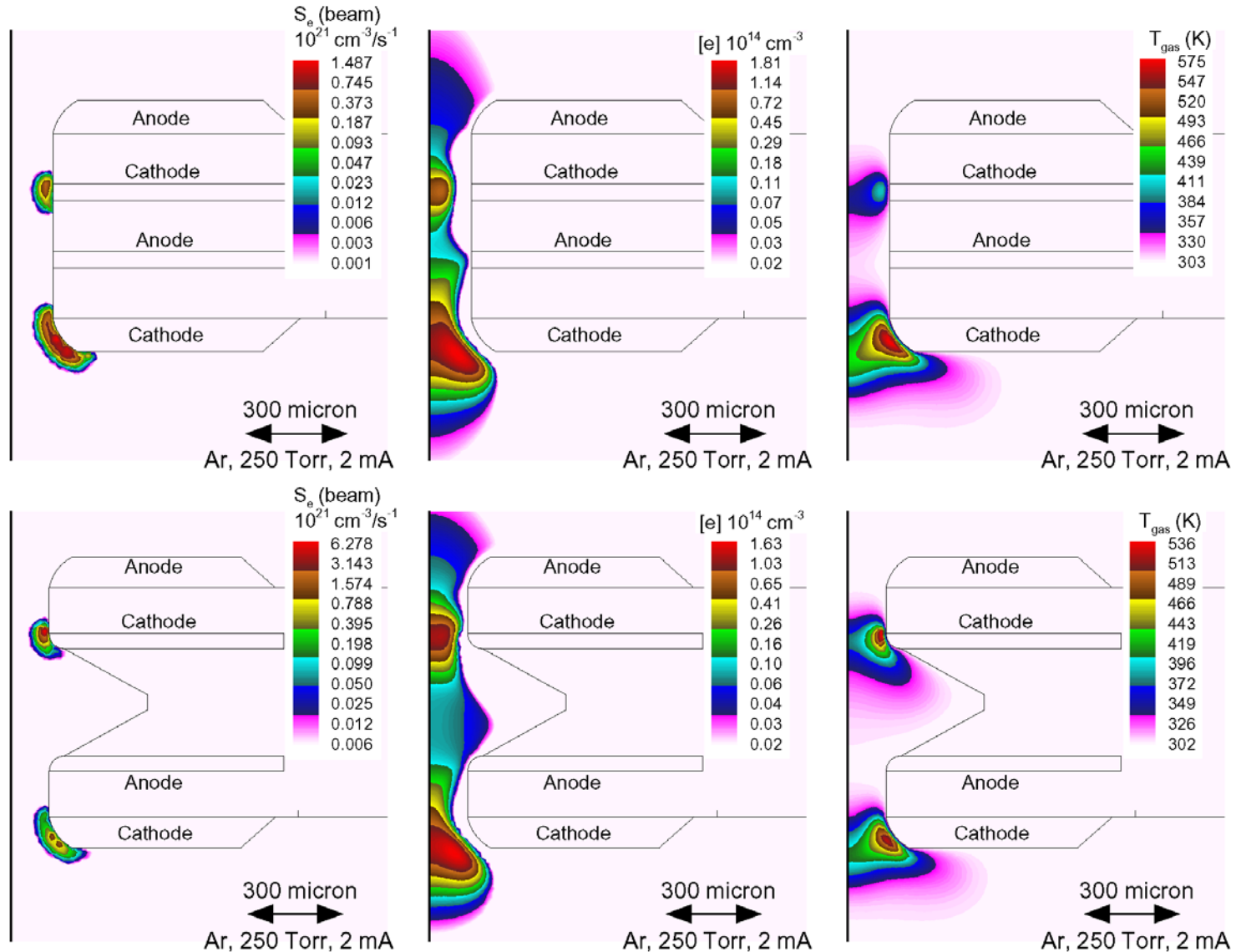


• 600 Torr Ne.

University of Illinois
Optical and Discharge Physics

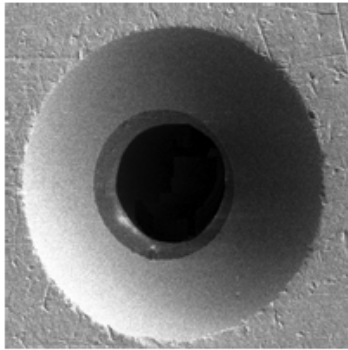
EXAMPLES OF 2-STAGE MDs

- Design affects gas heating, rarefaction; range and influence of secondary electrons and division of current.

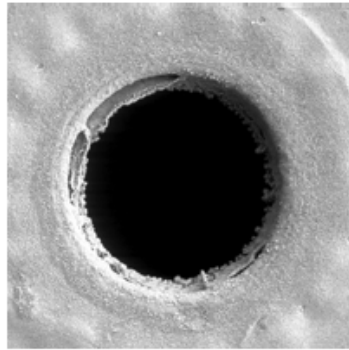


DESIGNING MDs AS VISIBLE SOURCES: AGING

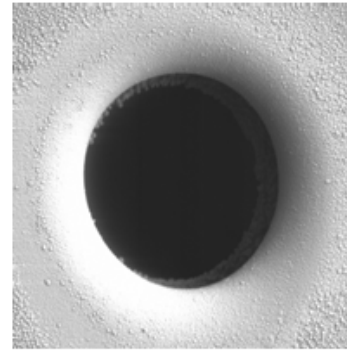
- As MDs age with use, critical dimensions and material properties (such as secondary emission coefficients) often change.
- Modeling is valuable in the design process to determine the sensitivity of optical properties to aging related changes in device parameters.



New



Anode (aged)



Cathode (aged)

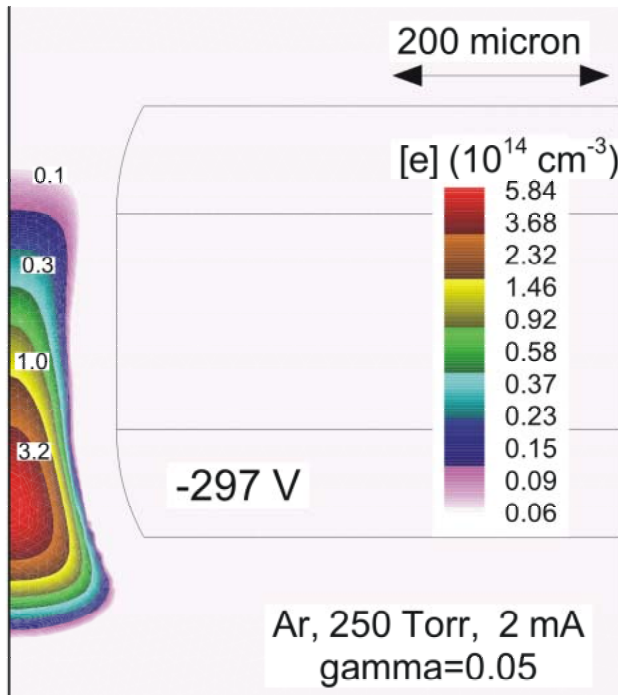
Ar, 380 Torr, 5 mA, 10 hours

- Ref: Maria Cristina Penache, Thesis, 2002

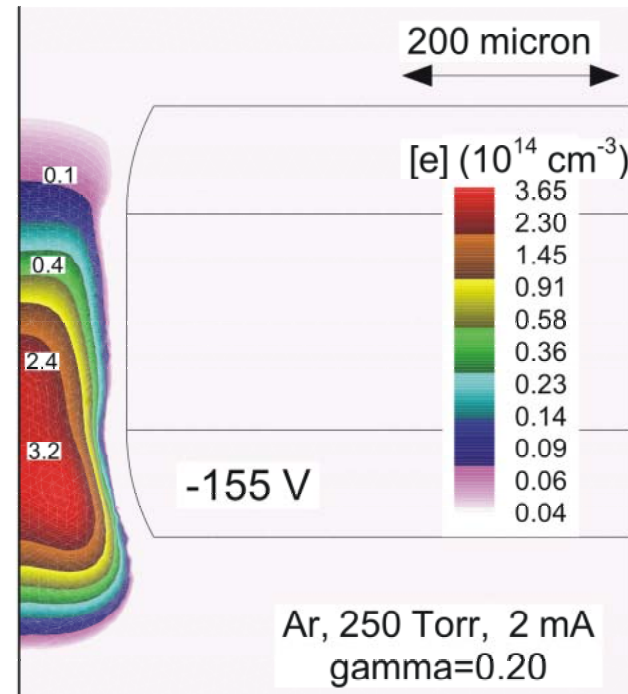
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SENSITIVITY TO γ (SECONDARY EMISSION): [e]

- The electron density increases with decreasing γ , a counter-intuitive result likely produced by more efficient ionization by the more energetic secondary electrons.



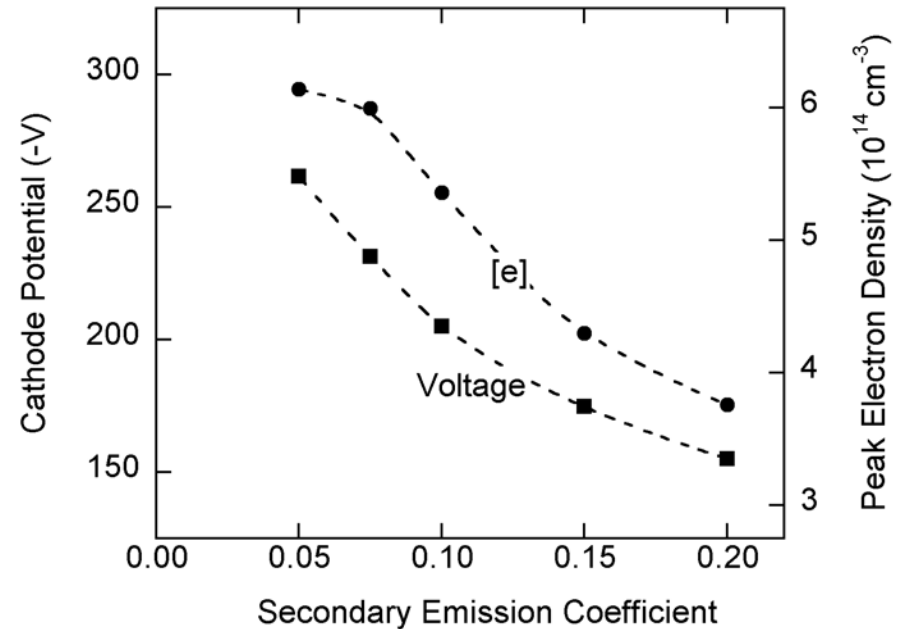
- $\gamma = 0.05$



- $\gamma = 0.20$

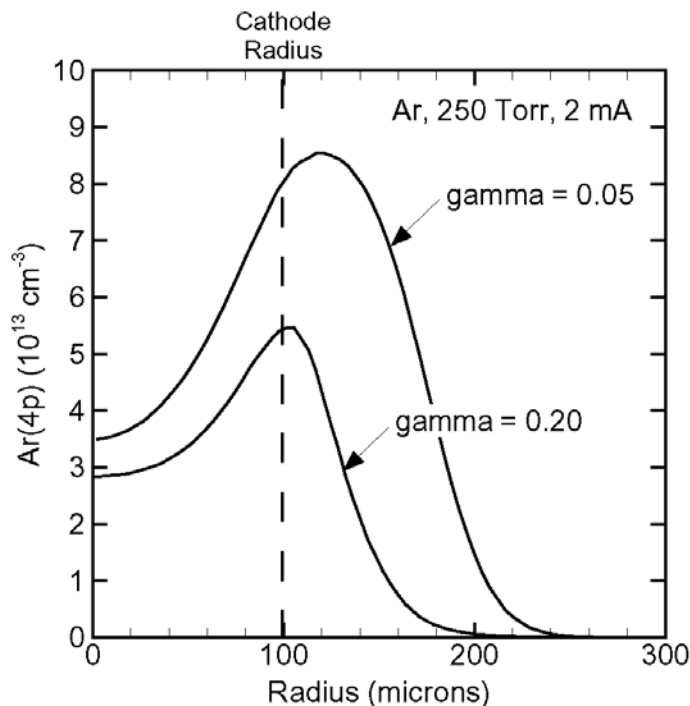
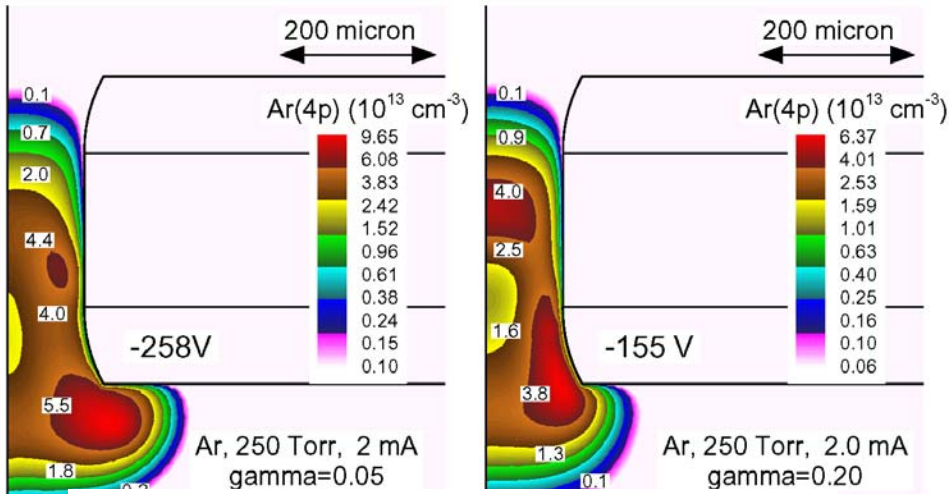
SENSITIVITY TO γ (SECONDARY EMISSION): VOLTAGE, [e]

- Voltage and peak electron density increases with decreasing γ to counter smaller flux of beam electrons which ionize efficiently.
- Power increases when holding current constant.



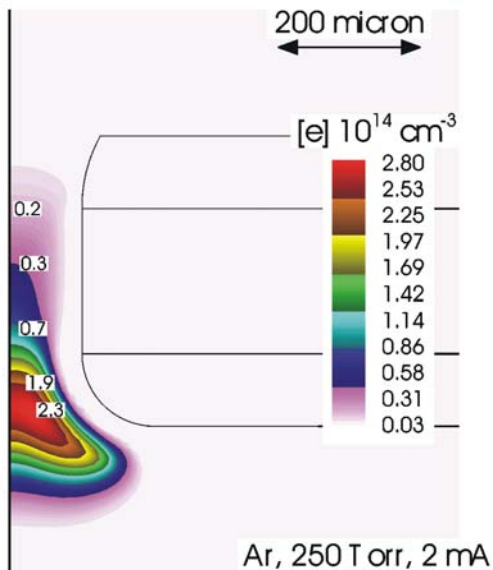
- Ar, 250 Torr, 2 mA

SENSITIVITY TO γ : VISIBLE EMISSION

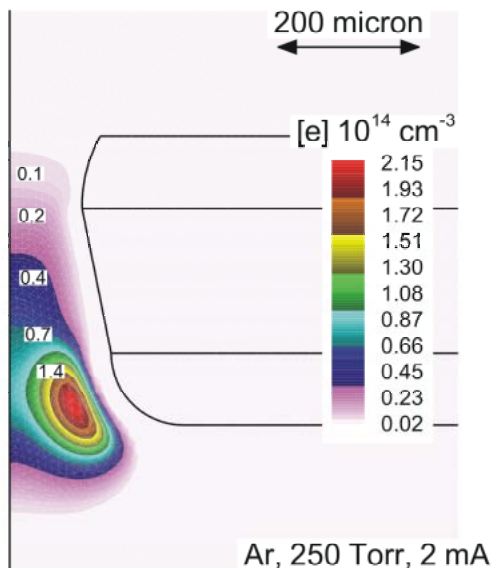


- **Visible emission increases as γ decreases, in part reflecting increase in power.**
- **Distribution of emission also shifts to being more dominated by beam electrons.**
- **Ar, 250 Torr, 2 mA**

SENSITIVITY TO CRITICAL DIMENSIONS: [e]



- **Straight**

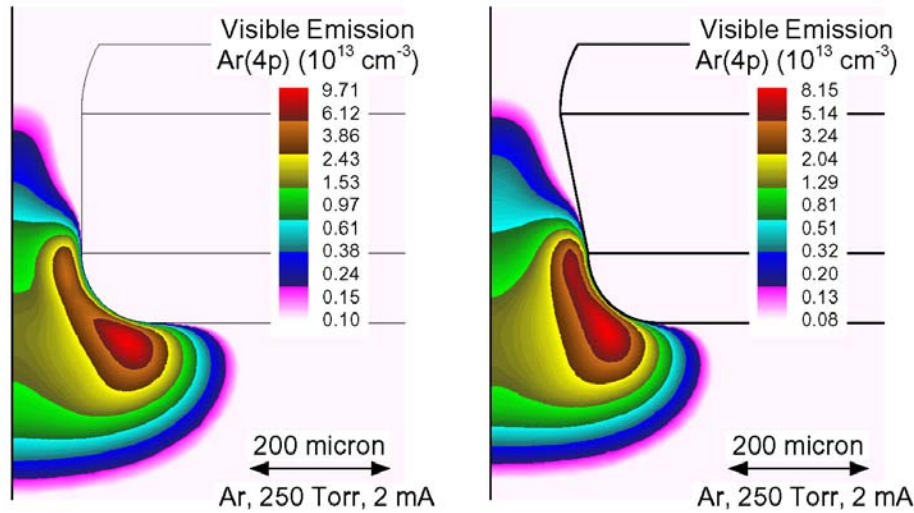


- **Tapered**

- Device-to-device variation in fabrication or erosion/wear during operation may change critical dimensions. How sensitive are operating characteristics?
- Contrast straight and tapered dielectrics.
- Peak electron density is higher and more distributed in straight MD.
- Ar, 250 Torr, 2 mA

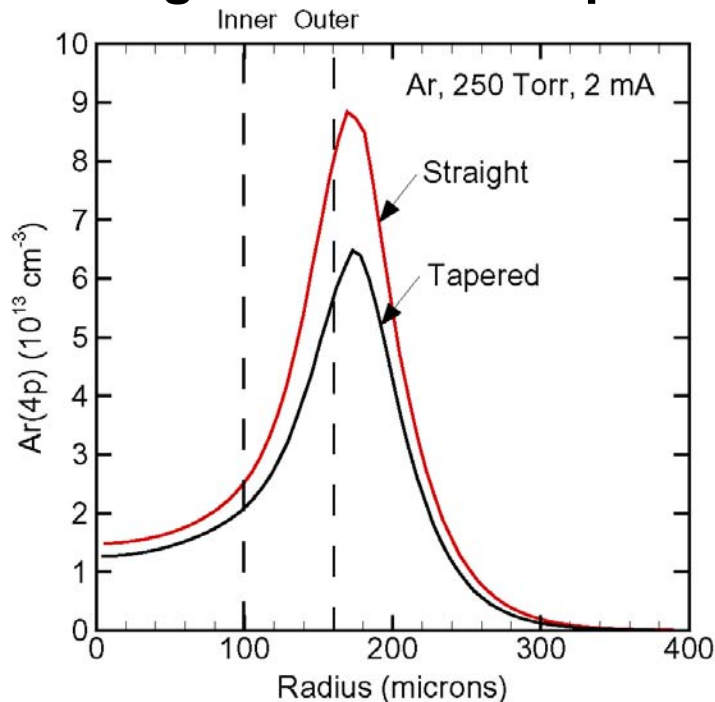
SENSITIVITY TO CRITICAL DIMENSIONS: VISIBLE EMISSION

- Magnitude of visible emission is sensitive to loss in critical dimension.
- Distribution is less sensitive.
- Robust designs are possible which are tolerant to erosion and loss of critical dimension.
- Ar, 250 Torr, 2 mA



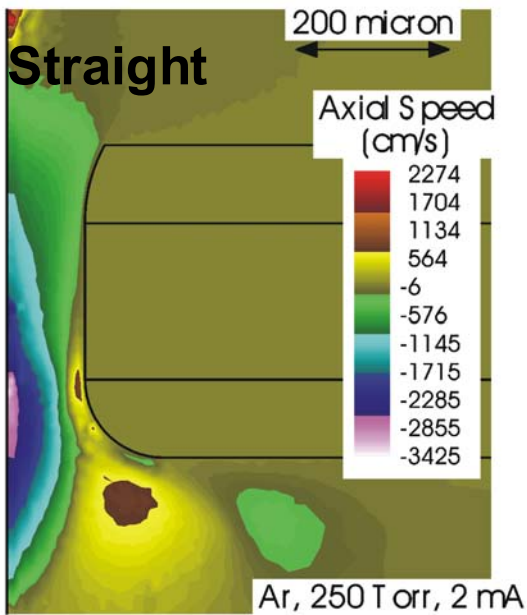
• Straight

• Tapered



SENSITIVITY TO CRITICAL DIMENSIONS : AXIAL FLOW

- **Straight**

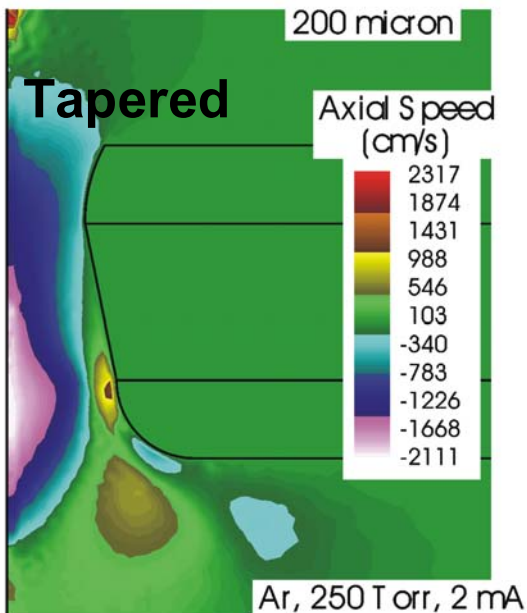


- Speed of (downward) axial flow produced by cataphoresis is $> 50\%$ higher in the less tapered MD.

- Higher current density, larger E/N, larger on-axis plasma density all contribute.

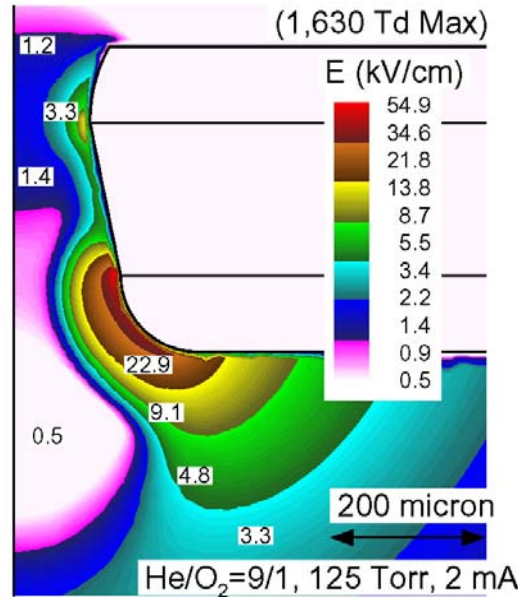
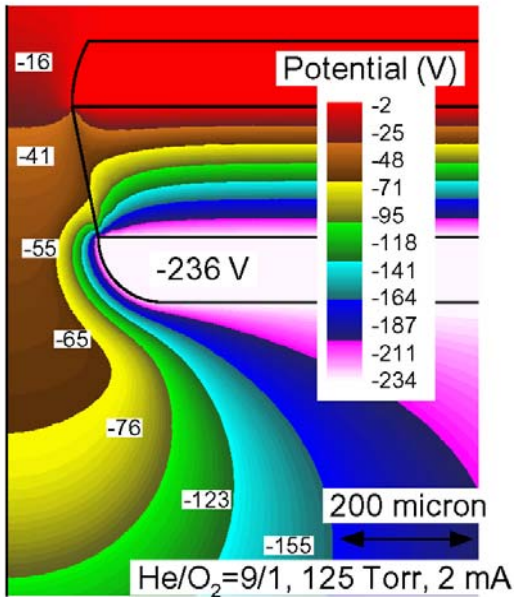
- Ar, 250 Torr, 2 mA

- **Tapered**



MD AS A RADICAL SOURCE: He/O₂

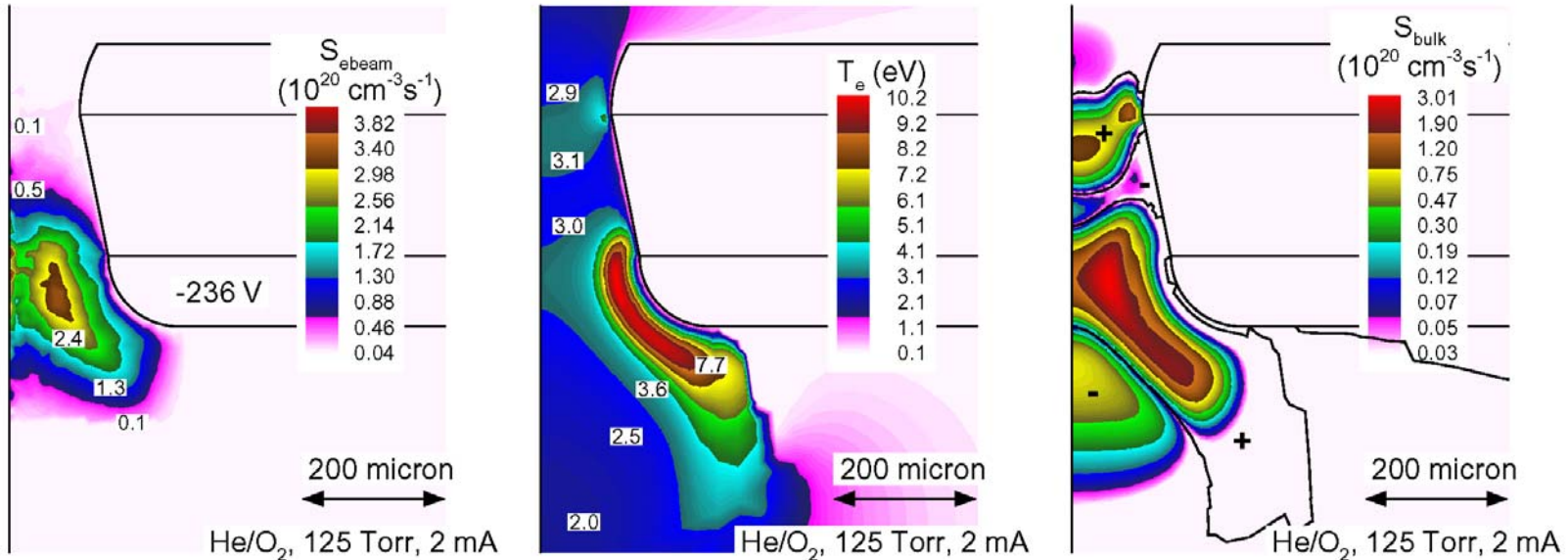
- Large current densities and intrinsically high gas flow makes MDs ideal for reactant generators. Demonstrate with electronegative He/O₂ mixture.



- Higher collisionality produces larger operating voltages, larger electric fields.

- He/O₂=90/10, 125 Torr, 2 mA

MD SUSTAINED IN He/O₂: ELECTRON SOURCES



• S(beam)

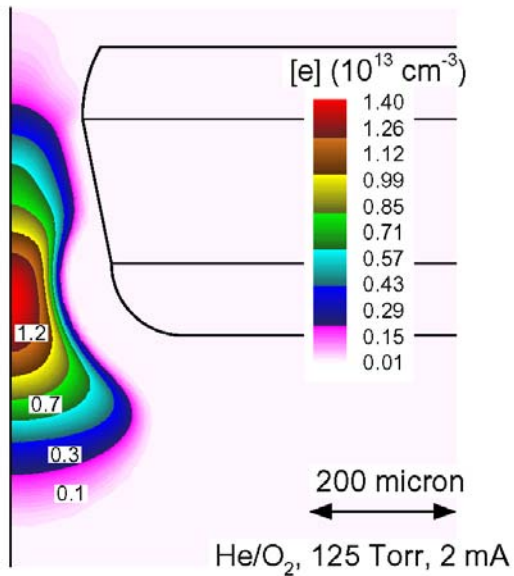
• T_e

• S(bulk)

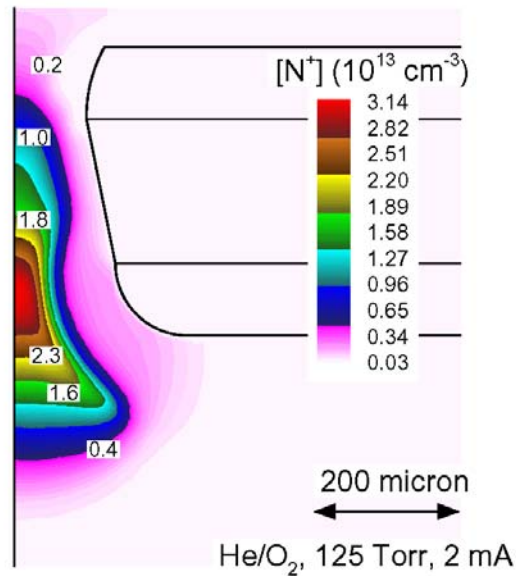
- Larger voltage enables efficiency beam ionization deep into plasma. Volumetric attachment produces distinct regions of positive and negative bulk sources

- He/O₂=90/10, 125 Torr, 2 mA

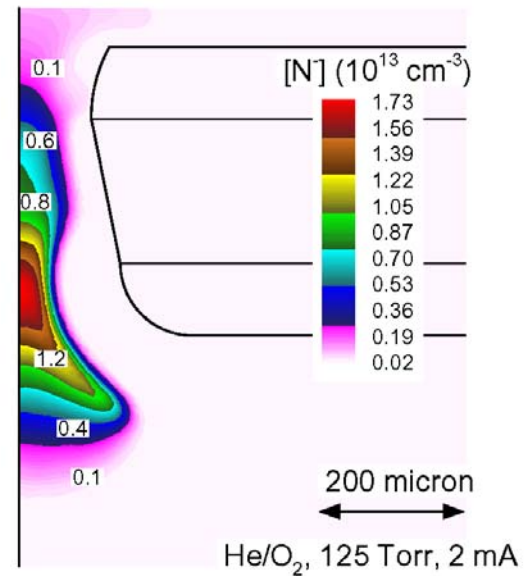
MD SUSTAINED IN He/O₂: ELECTRON, ION DENSITIES



• [e]



• [N⁺]

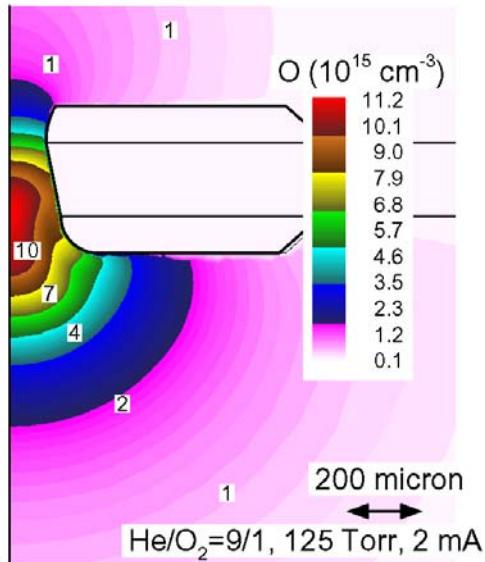


• [N⁻]

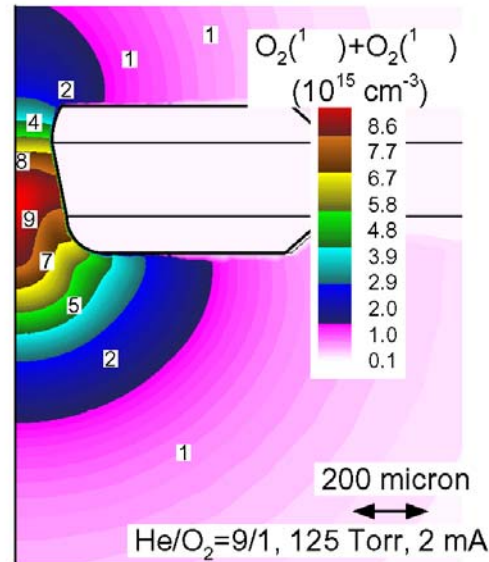
• Negative ions are dominated by O₂⁻ at pressures of 100s Torr.

• He/O₂=90/10, 125 Torr, 2 mA

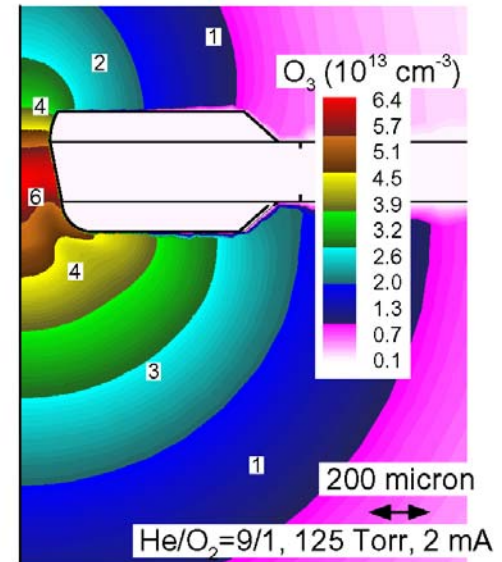
MD SUSTAINED IN He/O₂: RADICAL, EXCITED STATE DENSITIES



• [O]



• [O₂(¹Δ)]

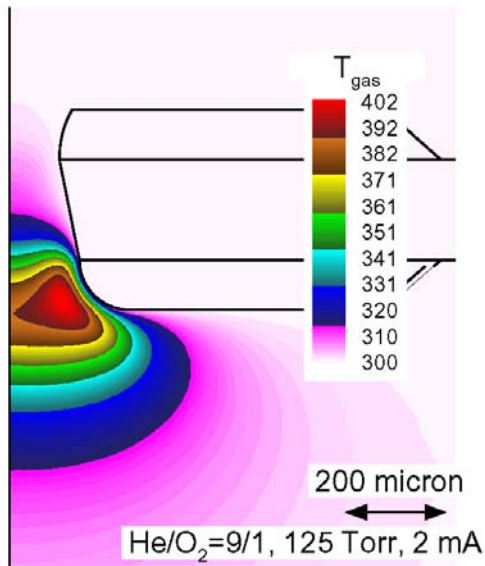


• [O₃]

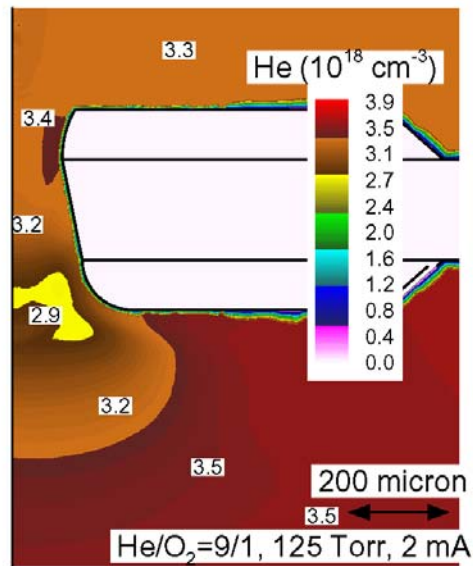
- The range of O atoms is limited by recombination and ozone formation. O₂(¹Δ) and O₃ are final products, having longer ranges.
- Cataphoresis induced flow preferentially ejects reactants downward.

• He/O₂=90/10, 125 Torr, 2 mA

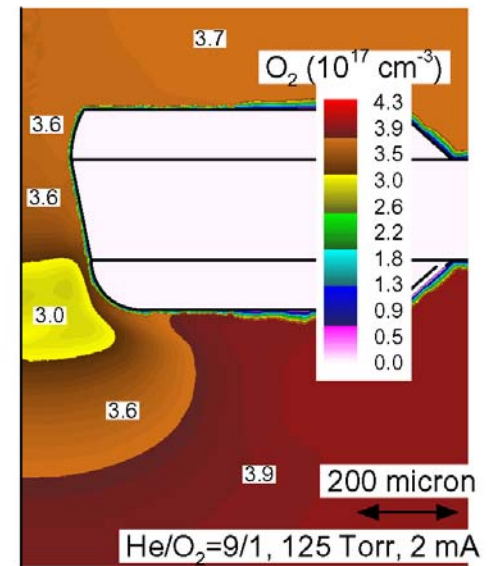
MD SUSTAINED IN He/O₂: FLOW PROPERTIES



- T(gas)



- [He]

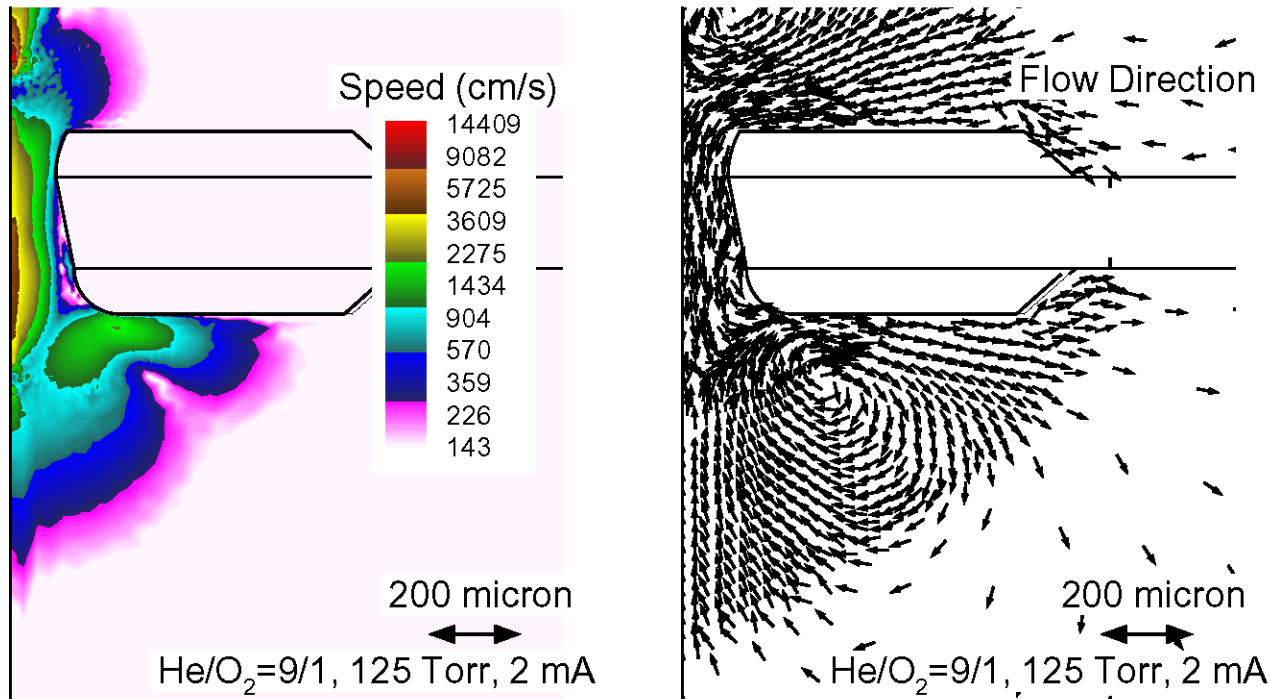


- [O₂]

- In spite of Frank-Condon heating, gas temperatures are lower (for a give current) than in argon due to higher thermal conductivity of He.

- He/O₂=90/10, 125 Torr, 2 mA

MD SUSTAINED IN He/O₂: FLOW PROPERTIES

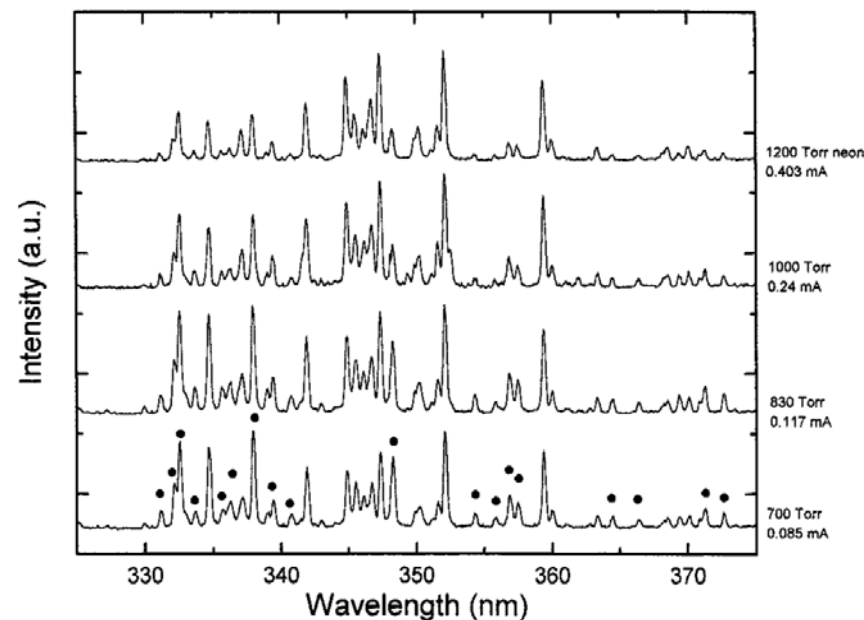
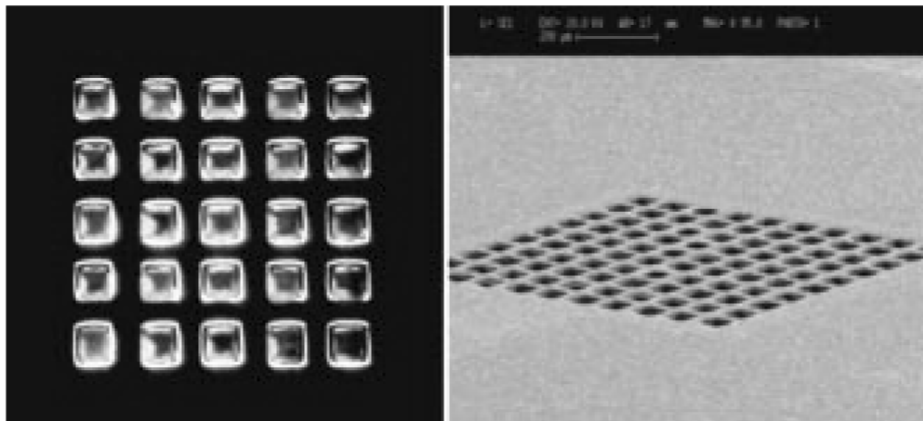
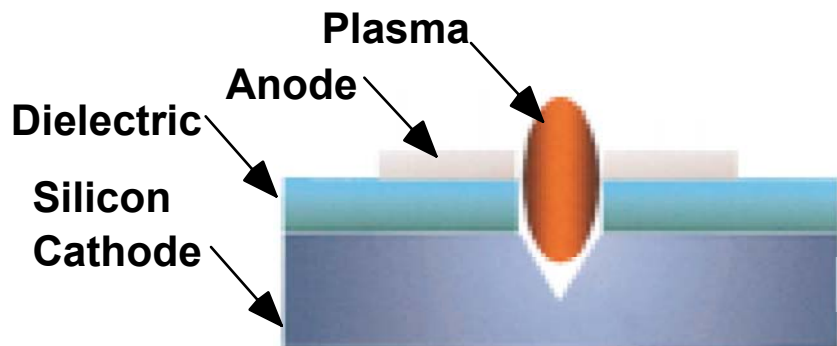


- Optimization of MDs as radical sources will require careful attention to flow properties to maximize delivery of reactants.

- He/O₂=90/10, 125 Torr, 2 mA

PYRAMIDAL MICRODISCHARGE DEVICES

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

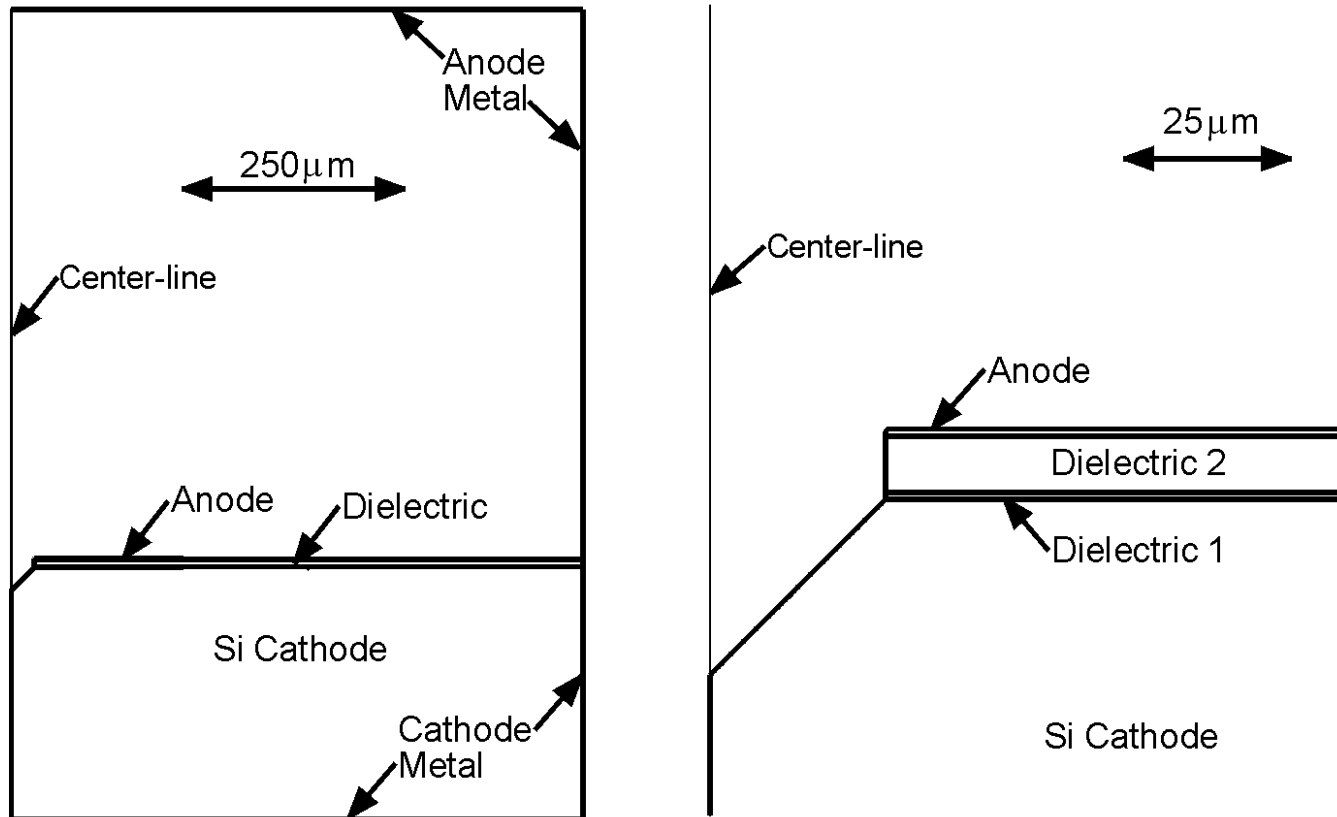


- S.-J. Park, et al., J. Sel. Topics Quant. Electron 8, 387 (2002); Appl. Phys. Lett. 78, 419 (2001).

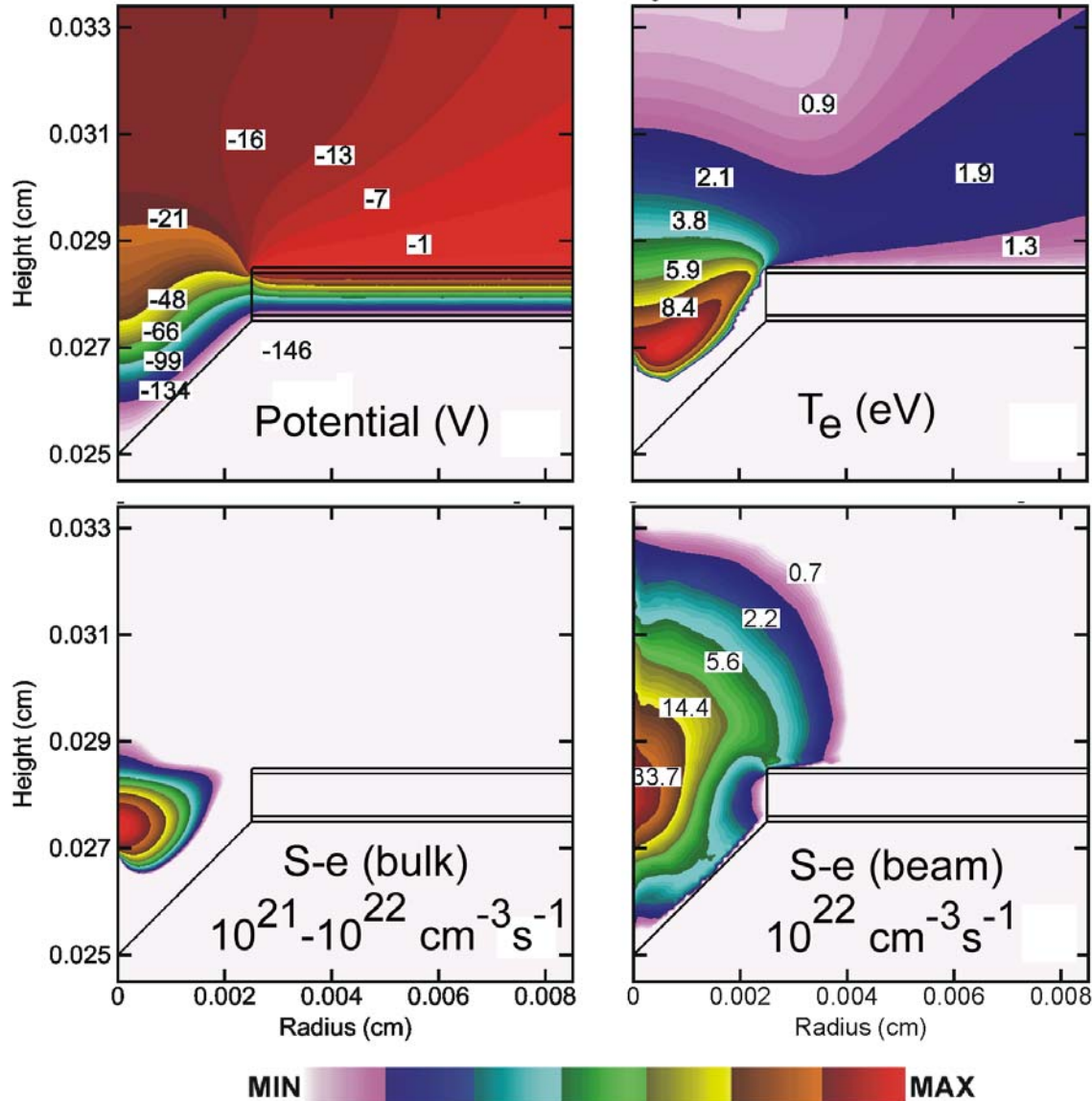
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MODEL GEOMETRY: Si PYRAMID MICRODISCHARGE

- Investigations of a cylindrically symmetric Si pyramid microdischarge were performed.



BASE CASE: Ne, 600 Torr, 50 μm DIAMETER



- Optimum operation produces large enough charge density to warp electric potential into cathode well.

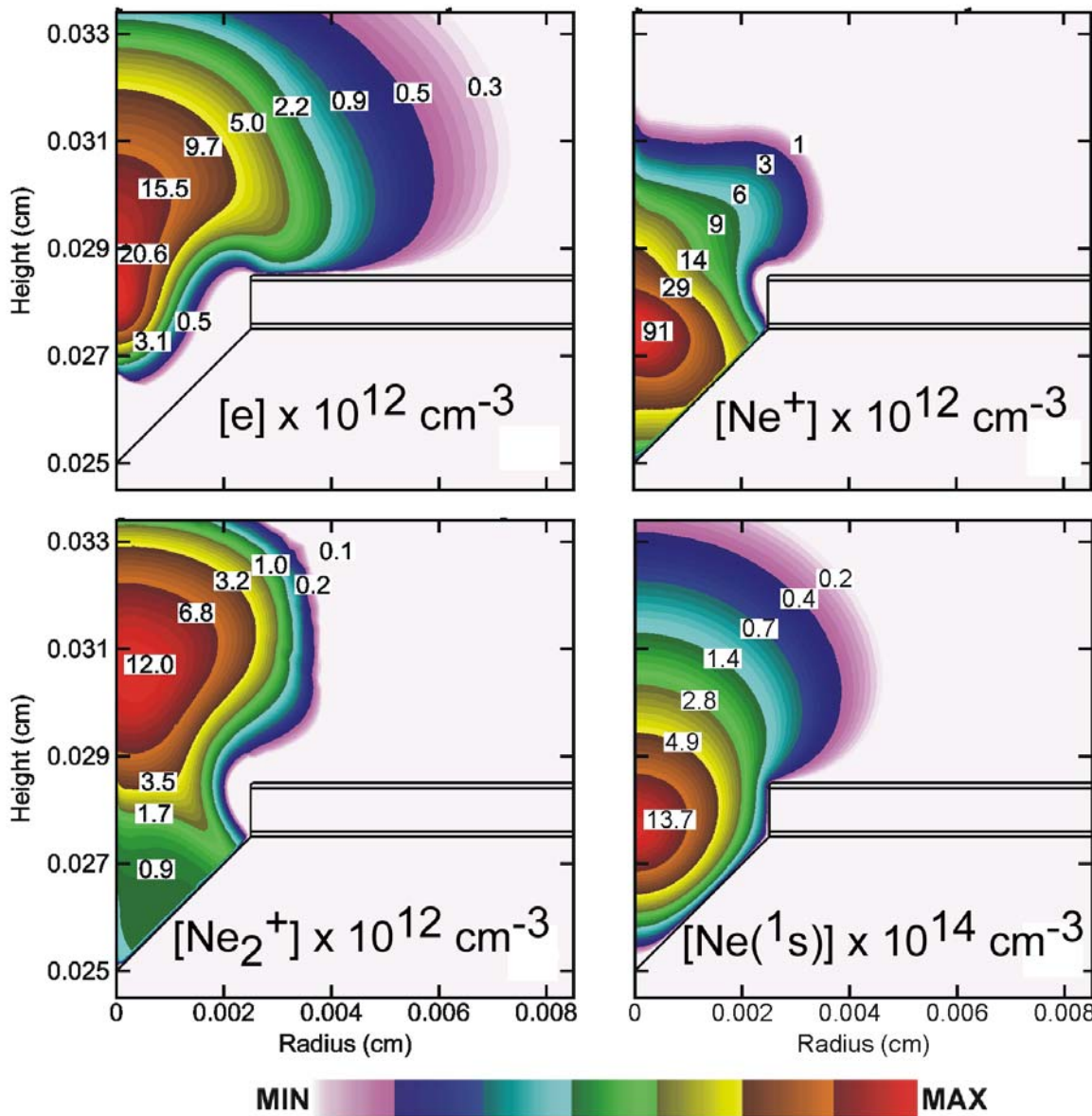
- In spite of large T_e , ionization is dominated by beam electrons

- Ne, 600 Torr, 50 μm ,
200 V, 1 $\text{M}\Omega$

BASE CASE: Ne, 600 Torr 50 μm DIAMETER

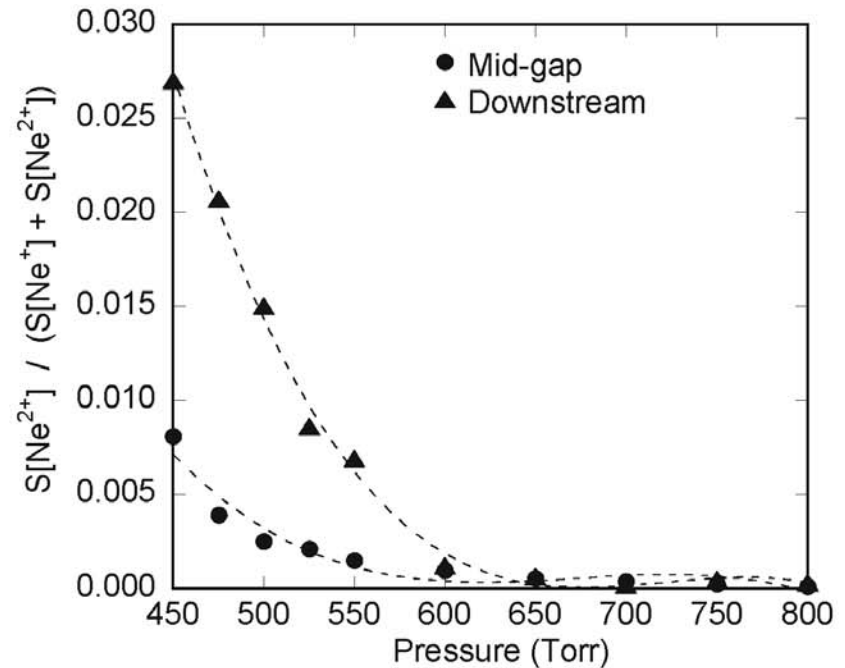
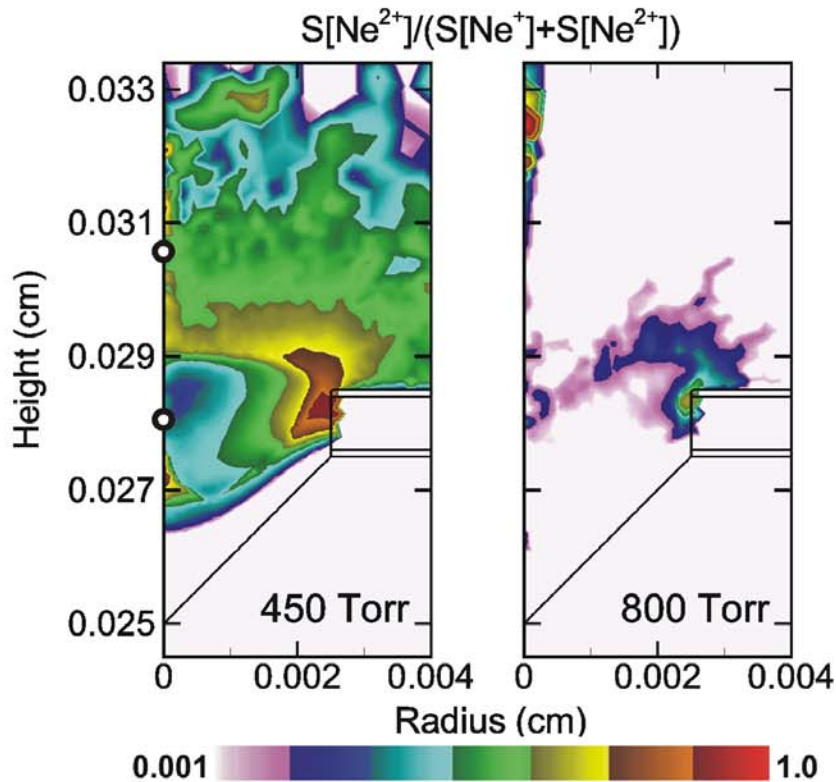
- There is essentially no region of quasi-neutrality or which is positive column-like.
- Monomer and dimer ions are segregated.
- Excited state densities $> 10^{15} \text{ cm}^{-3}$ rival macroscopic devices
- Ne, 600 Torr, 50 μm , 200 V, 1 $\text{M}\Omega$

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TRANSITION TO NEGATIVE-GLOW BEHAVIOR

- Although geometry precludes true hollow cathode behavior, negative glow behavior sets in at lower pressures.
- Characterize negative glow by $S[\text{Ne}^{2+}] / (S[\text{Ne}^+] + S[\text{Ne}^{2+}])$

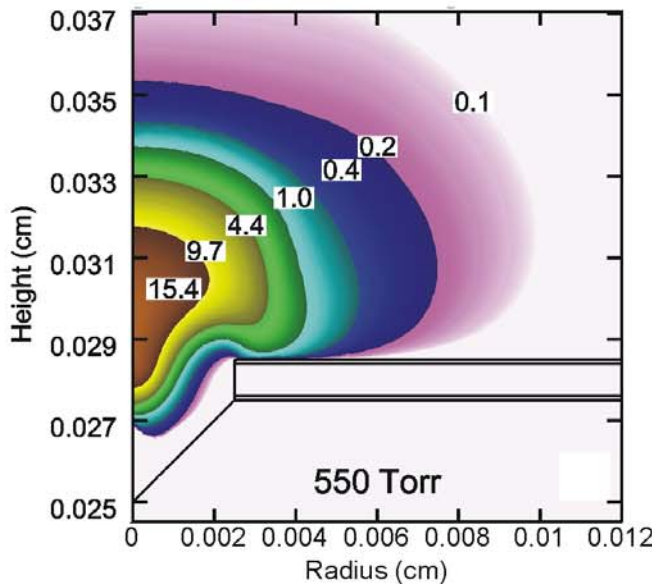


- Ne, 50 μm diameter, 200 V, 1 M Ω

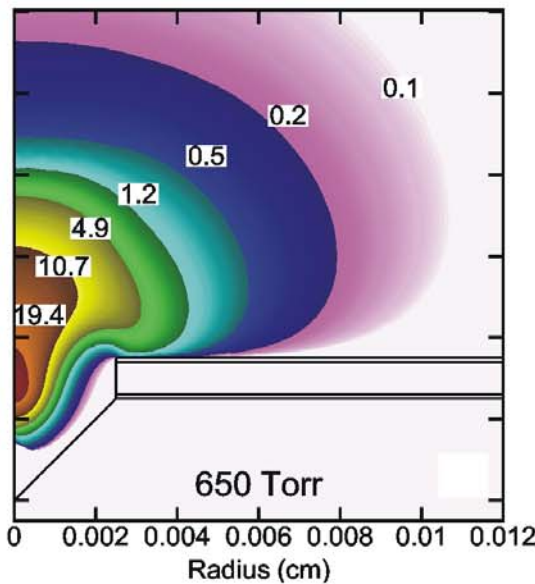
SCALING WITH PRESSURE: PLASMA PROPERTIES

- Over a range of pressures that $V(\text{applied})$ and $R(\text{ballast})$ can be constant, confinement at higher pressures produces higher peak plasma densities.

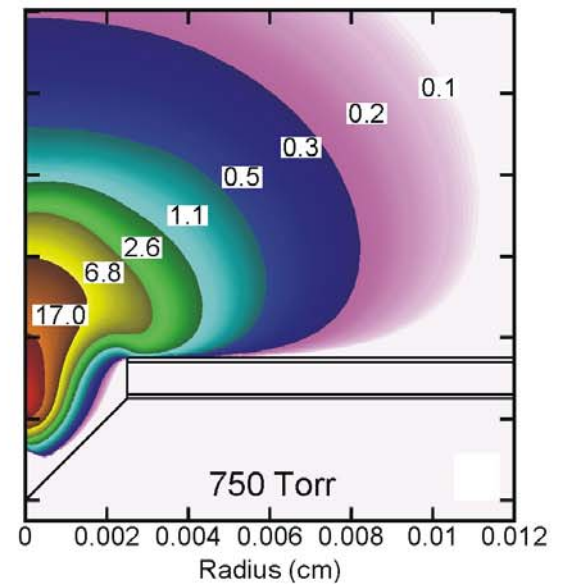
• $[e] \times 10^{12} \text{ cm}^{-3}$



• 550 Torr
[$2.1 \times 10^{13} \text{ cm}^{-3}$]



• 650 Torr
[$3.9 \times 10^{13} \text{ cm}^{-3}$]



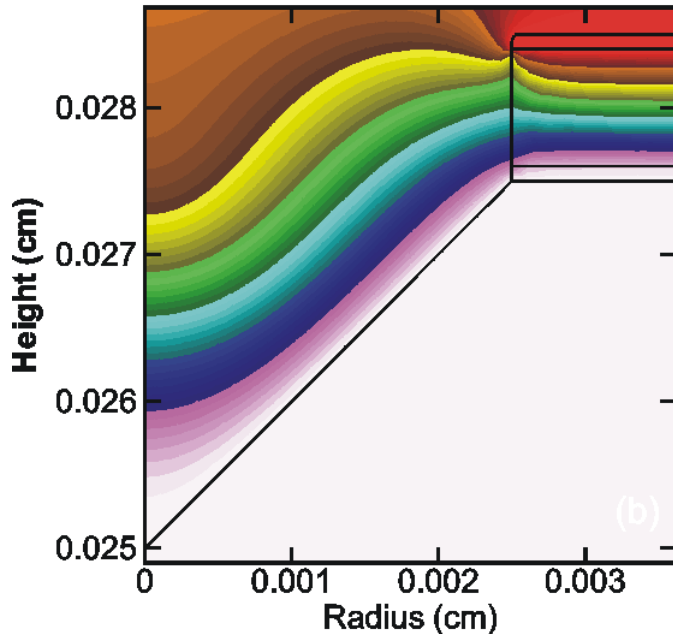
• 750 Torr
[$5.6 \times 10^{13} \text{ cm}^{-3}$]

• Ne, 50 μm diameter, 200V, 1 M Ω

SCALING CONSIDERATIONS: CATHODE FALL THICKNESS

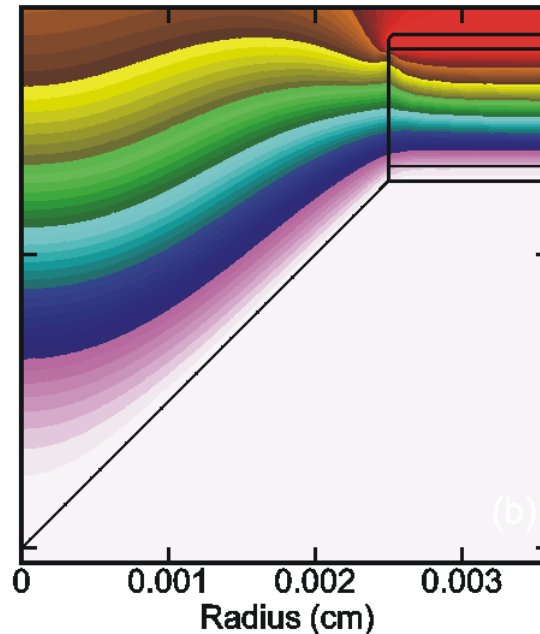
- In MDs, the cathode fall thickness may be commensurate with cavity size. Current density is therefore critical to scaling.

Potential [-147 to 0 V]



- -210 V, 1 M Ω
[e]= 4.9 x 10¹³ cm⁻³

Potential [-156 to 0 V]



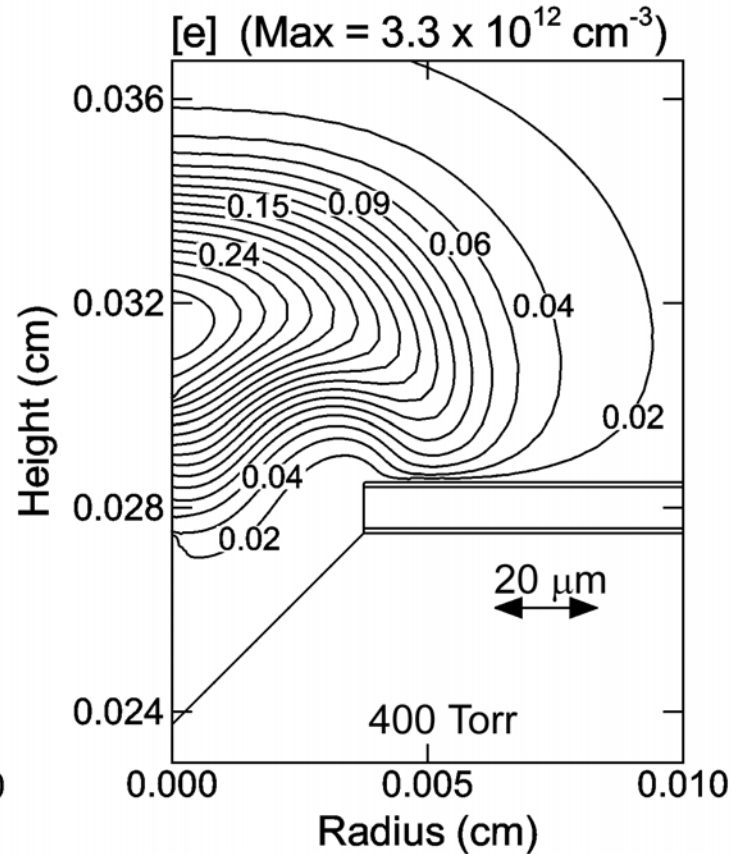
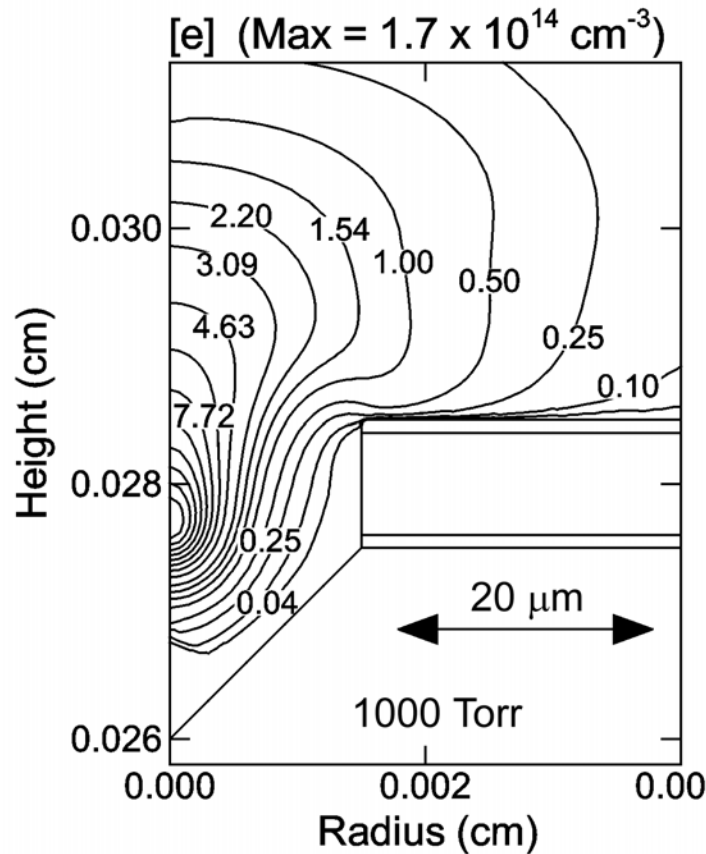
- -200 V, 1.75 M Ω
[e]= 5.3 x 10¹² cm⁻³

- Low j (and $[e]$) may result in cathode fall not being conformal to cathode.

- Ne, 50 μm diameter, 600 Torr

SCALING WITH SIZE: pd, BALLAST = CONSTANT

- Scaling while maintaining pd, V(applied) and R(ballast) constant results in a reduced j and [e] in the larger device. The plasma is not conformal to the cathode.

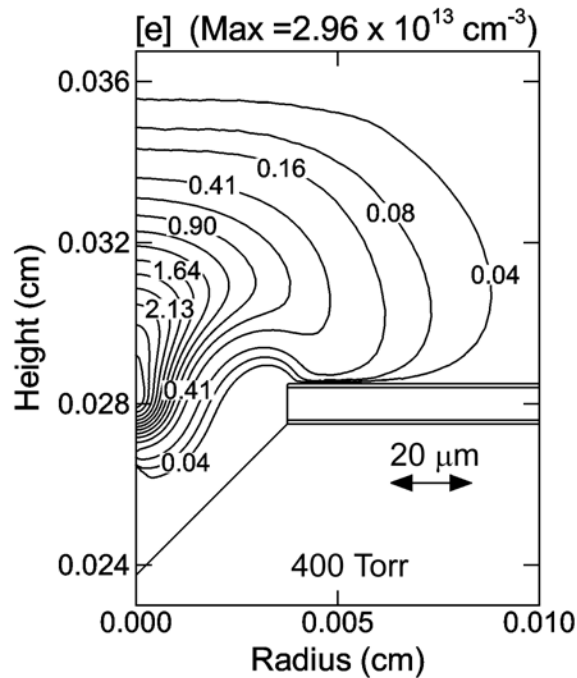


• Ne, -200 V, 1 MΩ

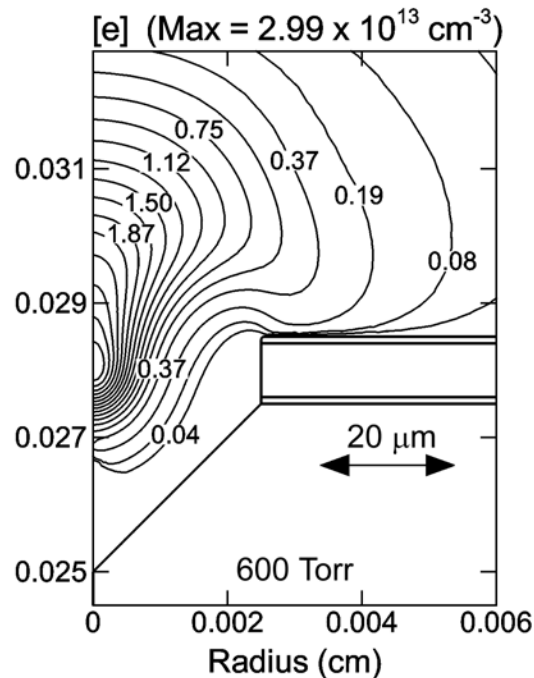
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SCALING WITH SIZE: $pd, j = \text{CONSTANT}$

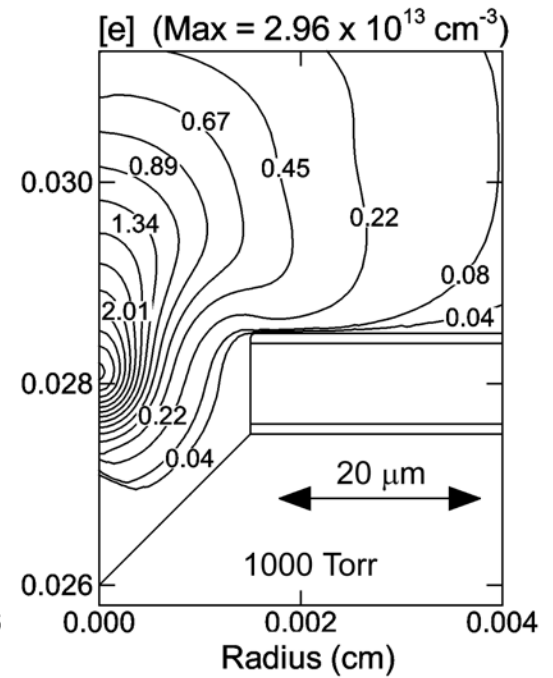
- Scaling while maintaining pd and j constant produces similar plasma densities and conformality to the cathode.



• 400 Torr



• 600 Torr



• 1000 Torr

• Ne, -200 V

CONCLUDING REMARKS

- MDs (even in a dc mode) are dynamic entities with strong coupling between electron and ion transport, gas dynamics and chemical processes.
- Subtle changes in geometry, physical parameters (e.g., secondary emission coefficient) can have profound impact on operating characteristics.
- There are significant differences in pd scaling between devices with $L > \text{Debye lengths (or cathode fall)}$ and $L < \lambda, d$.
- As MDs age with use, critical dimensions and material properties (such as secondary emission coefficients) often change.
- Modeling is valuable in the design process to determine the sensitivity of operating characteristics to aging related changes in device parameters.