MODELING OF COLLISIONAL, LOW TEMPERATURE PLASMAS: FUNDAMENTALS AND APPLICATIONS

Mark J. Kushner
University of Illinois
Department of Electrical and Computer Engineering
Urbana, IL 61801

mjk@uiuc.edu http://uigelz.ece.uiuc.edu

June 2000

ACKNOWLEDGMENTS

- **Former and Current Members of the Computational Optical and Discharge Physics Group**

Students

Jeanne Balbach
Paul Barnes
Seung Choi
Daniel W. Cronin
John V. Dicarlo
Rajesh Dorai
Diane Evans
Ann C. Gentile
Michael Grapperhaus
Michael J. Hartig
Robert J. Hoekstra
Fred Y. Huang
Helen H. Hwang
Ron L. Kinder
Brian M. Lay
Junqing Lu
Michael J. McCaughey
Hoyoung Pak
Timothy Peck
Mustafa Pinbarsi
Arvind Sankaran
Todd Saunders
Jong Shon
Daniel Storch
Pramod Subramonium
Phillip J. Stout
Yilin Weng
Xudong "Peter" Xu
G. Y. Yeom
Da Zhang

Post-Doctoral Fellows

Wenli Z. Collison
Eric R. Keiter
Tom Moratz
Irene Peres
Shahid Rauf
Mieko Ohwa
Timothy J. Sommerer
Wen-yi Tan
Trudy van der Straaten
Peter L. G. Ventzek

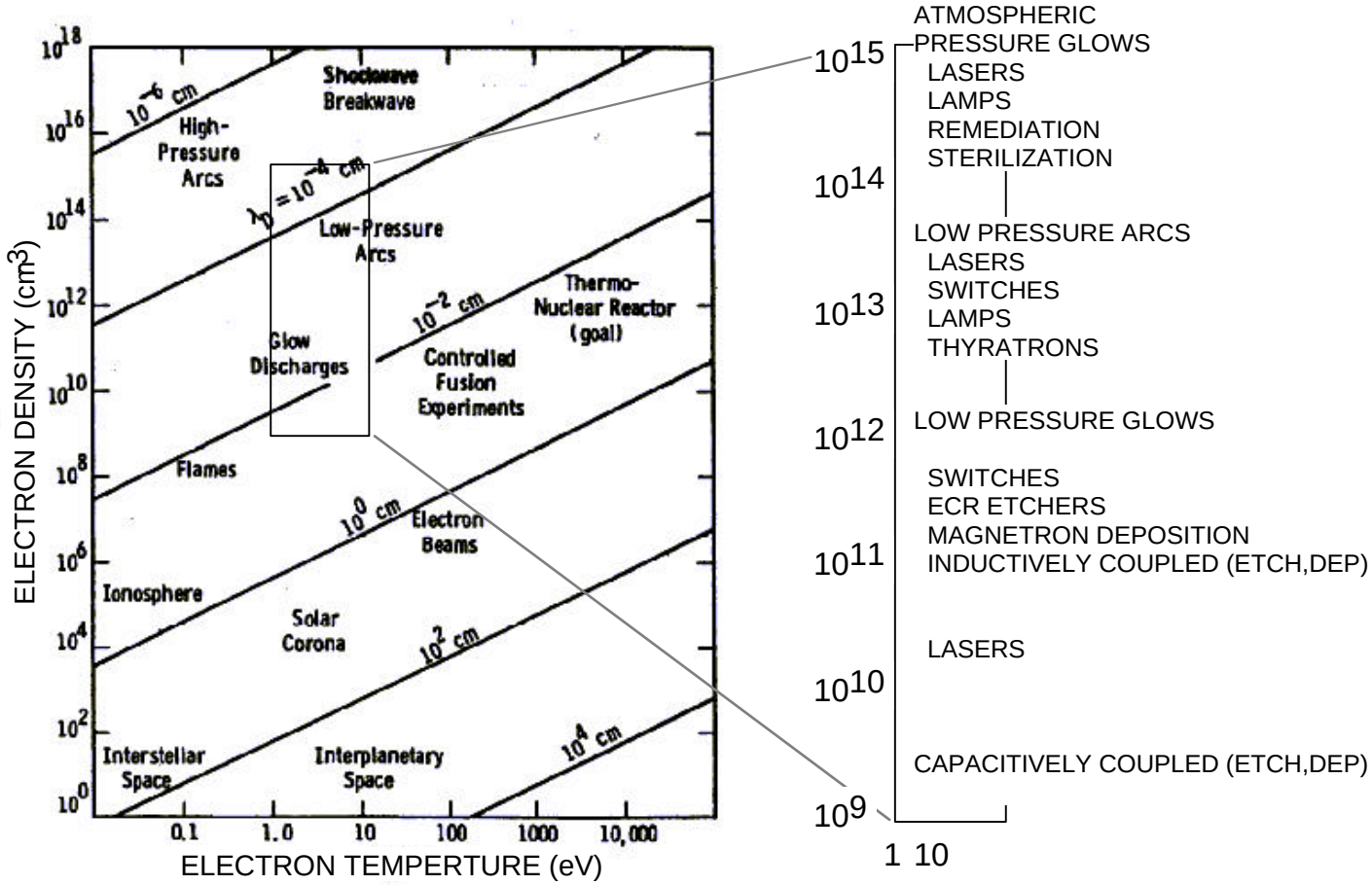
AGENDA

- Role of collisional plasmas in high technology manufacturing.
- Role of modeling in development and analysis of plasma tools.
- Historical perspective of model development.
- Examples of the use of modeling in equipment design.
- Concluding remarks.

University of Illinois
Optical and Discharge Physics

COLLISIONAL, LOW TEMPERATURE PLASMAS

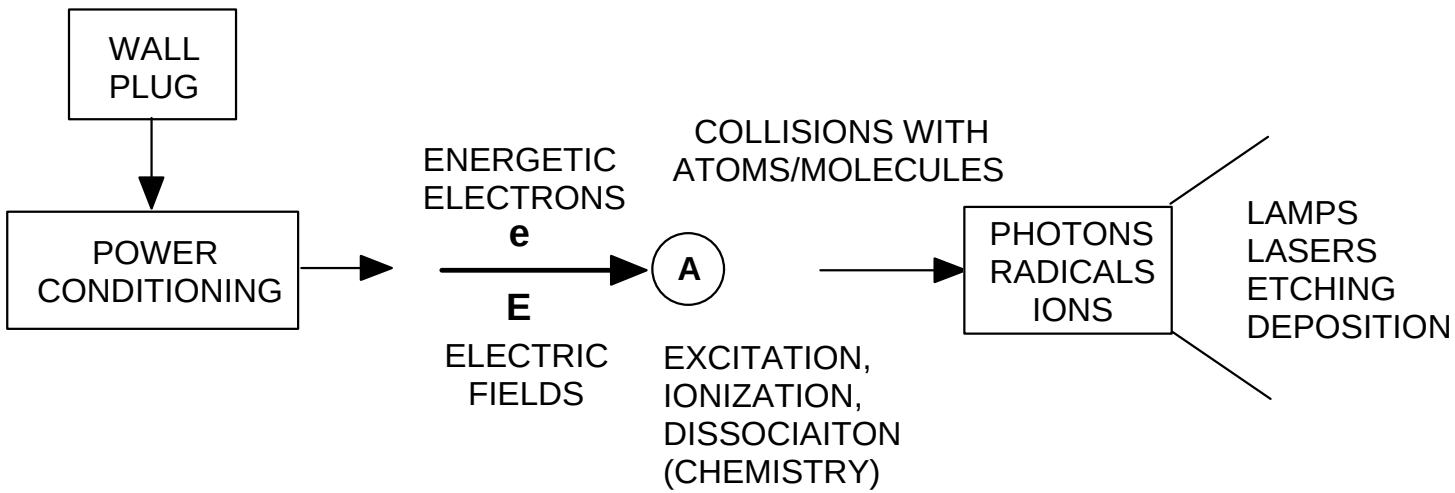
- **The plasmas of interest are low temperature (1-10 eV), partially ionized ([e]/N = 10^{-6}-10^{-2}) where electron collisions with neutrals (usually) dominate over collisions with ions (or other electrons).**



COLLISIONAL, LOW TEMPERATURE PLASMAS

- **These systems are the plasmas of everyday technology, "eV physics"**

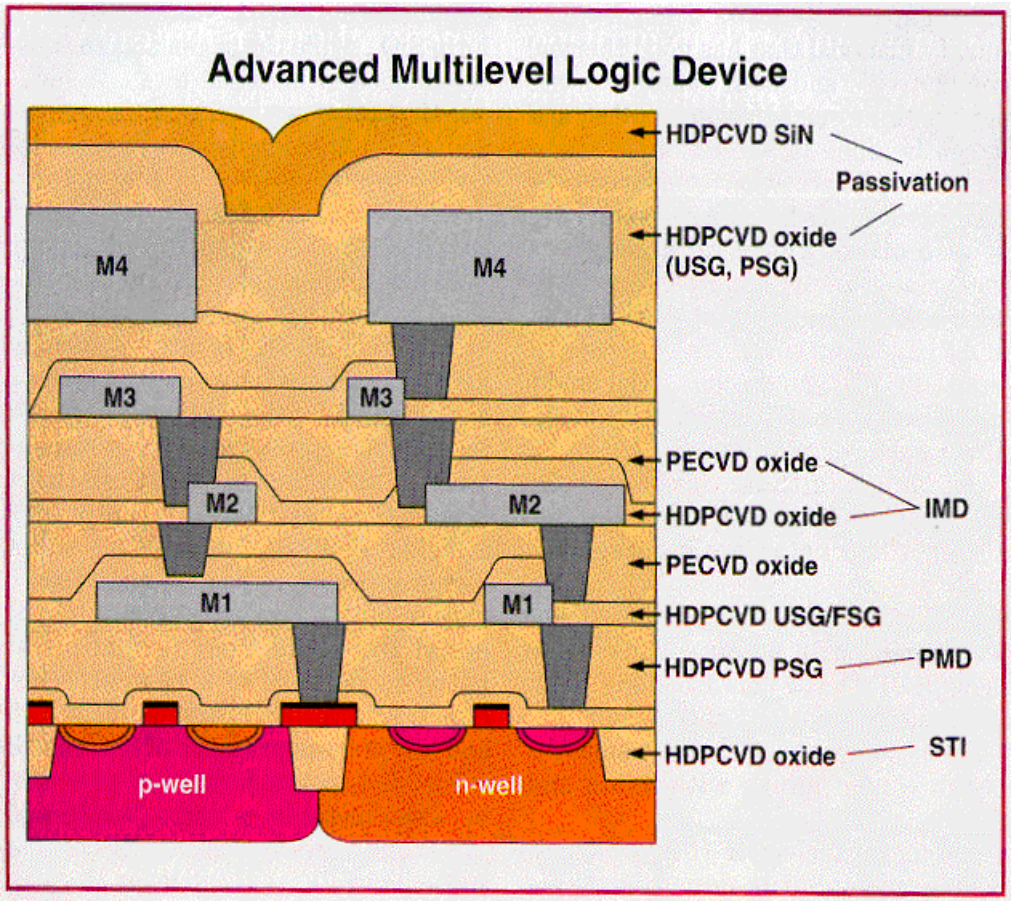
- **Electrons act as a mechanism to transfer power from the "wall plug" to the internal modes of atoms and molecules to "make a product".**

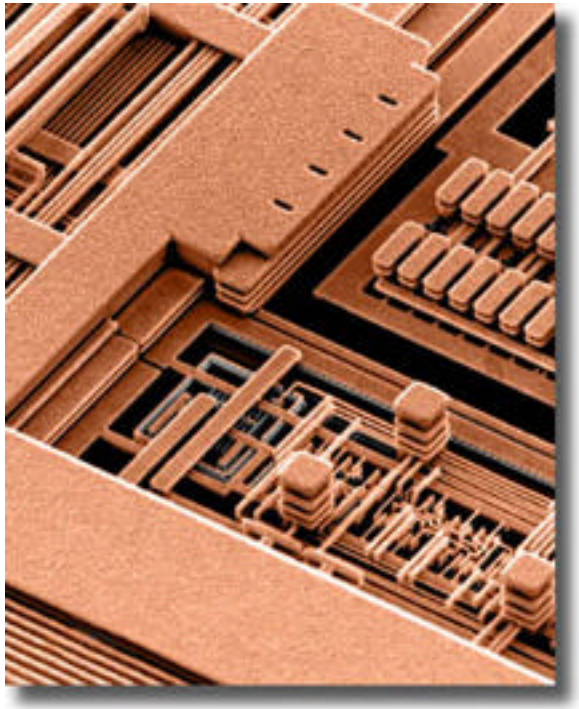


- **As a consequence, it is often difficult to separate the study of low temperature, partially ionized plasmas from the technology for which they are used.**

PLASMAS AND MICROELECTRONICS FABRICATION

- **The microelectronics industry is tasked with economically producing devices of increasing complexity (PIII >10^7 transistors) and shrinking size (0.13 μm).**





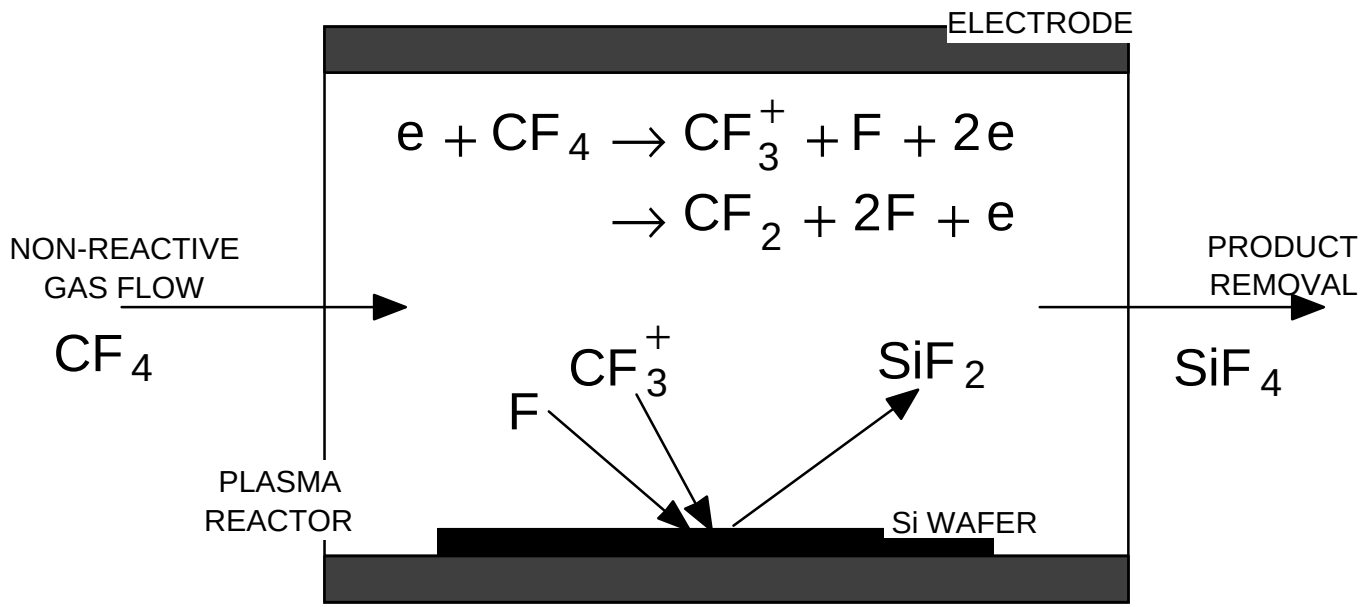
Ref: IBM Microelectronics

- **These innovations are enabled by low temperature, collisional plasmas.**

PLASMAS IN MICROELECTRONICS FABRICATION

- **Plasmas play a dual role in microelectronics fabrication....**

- **First, electron impact on otherwise unreactive gases produces neutral radicals and ions. That is, electrons are a power transfer medium.**

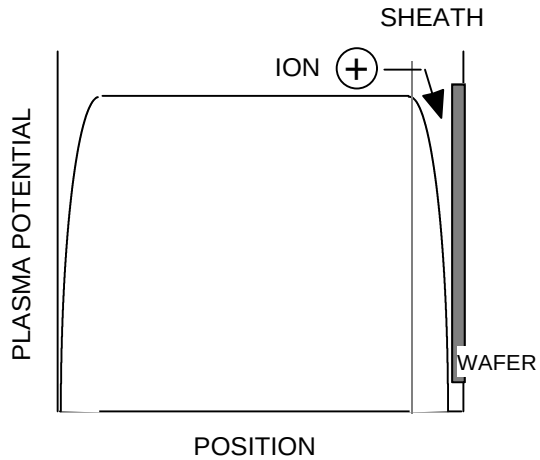


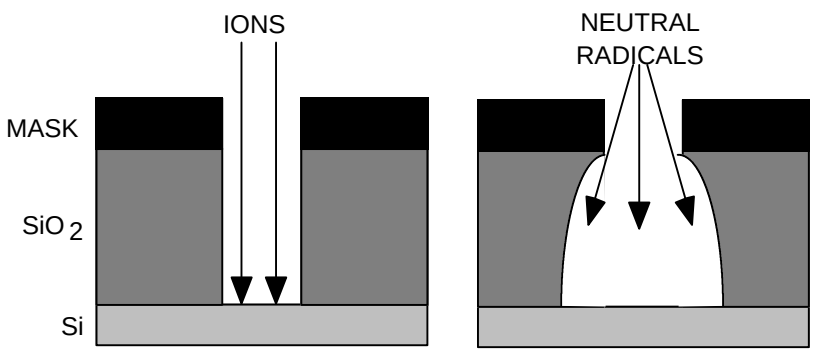
- **These active species drift or diffuse to the wafer where they remove or deposit materials.**

University of Illinois
Optical and Discharge Physics

PLASMAS IN MICROELECTRONICS FABRICATION

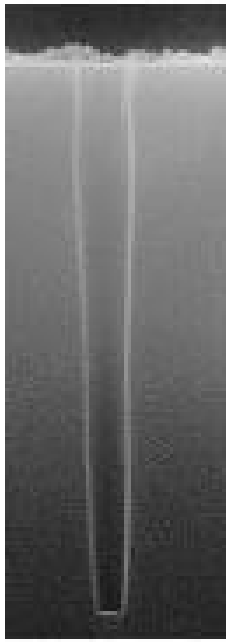
- **Second, ion acceleration in sheaths delivers directed activation energy to surfaces which enables fine features to be fabricated having extreme and reproducable tolerances.**





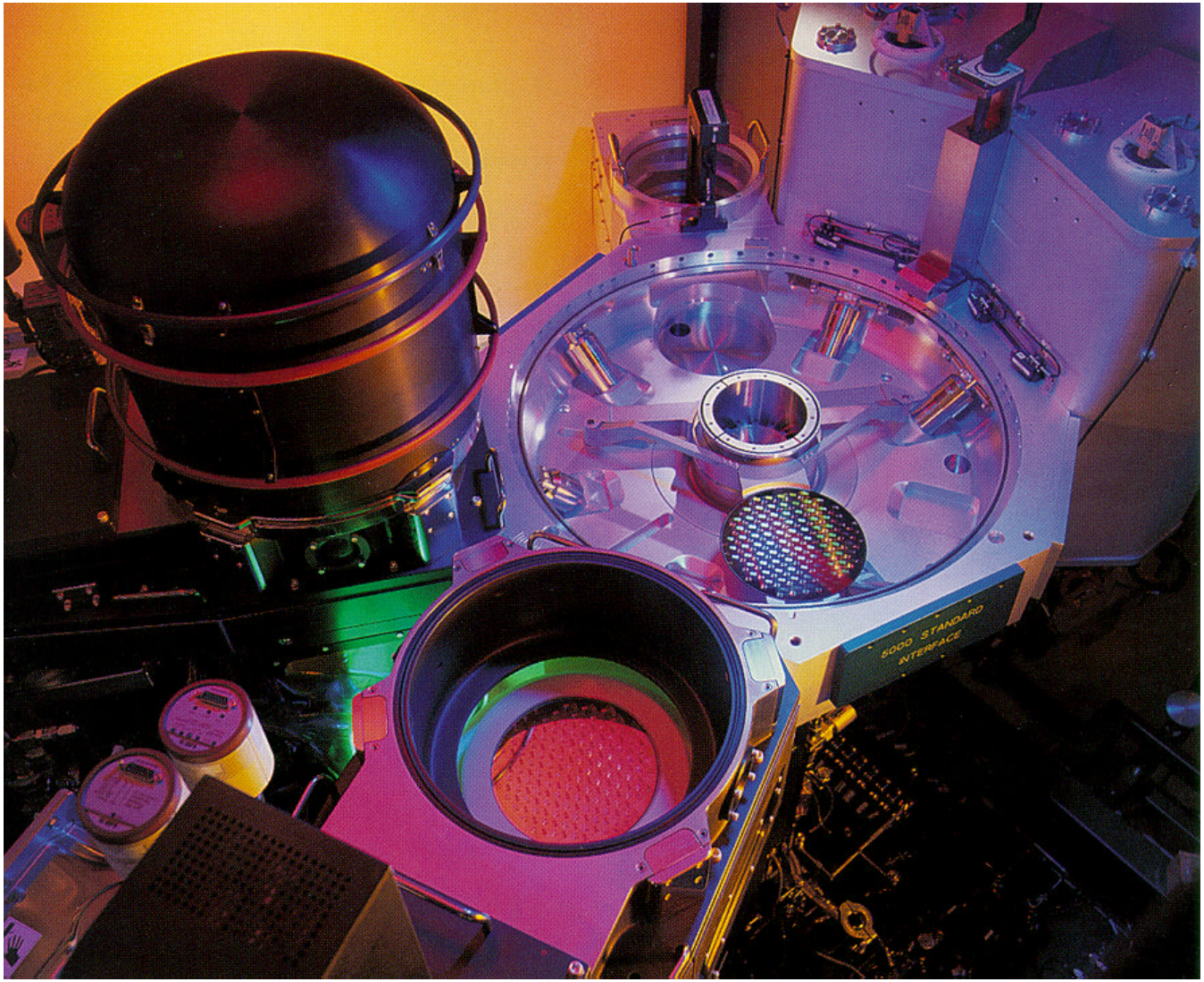
• Ion Assisted Etching

• Neutral Dominated Etching

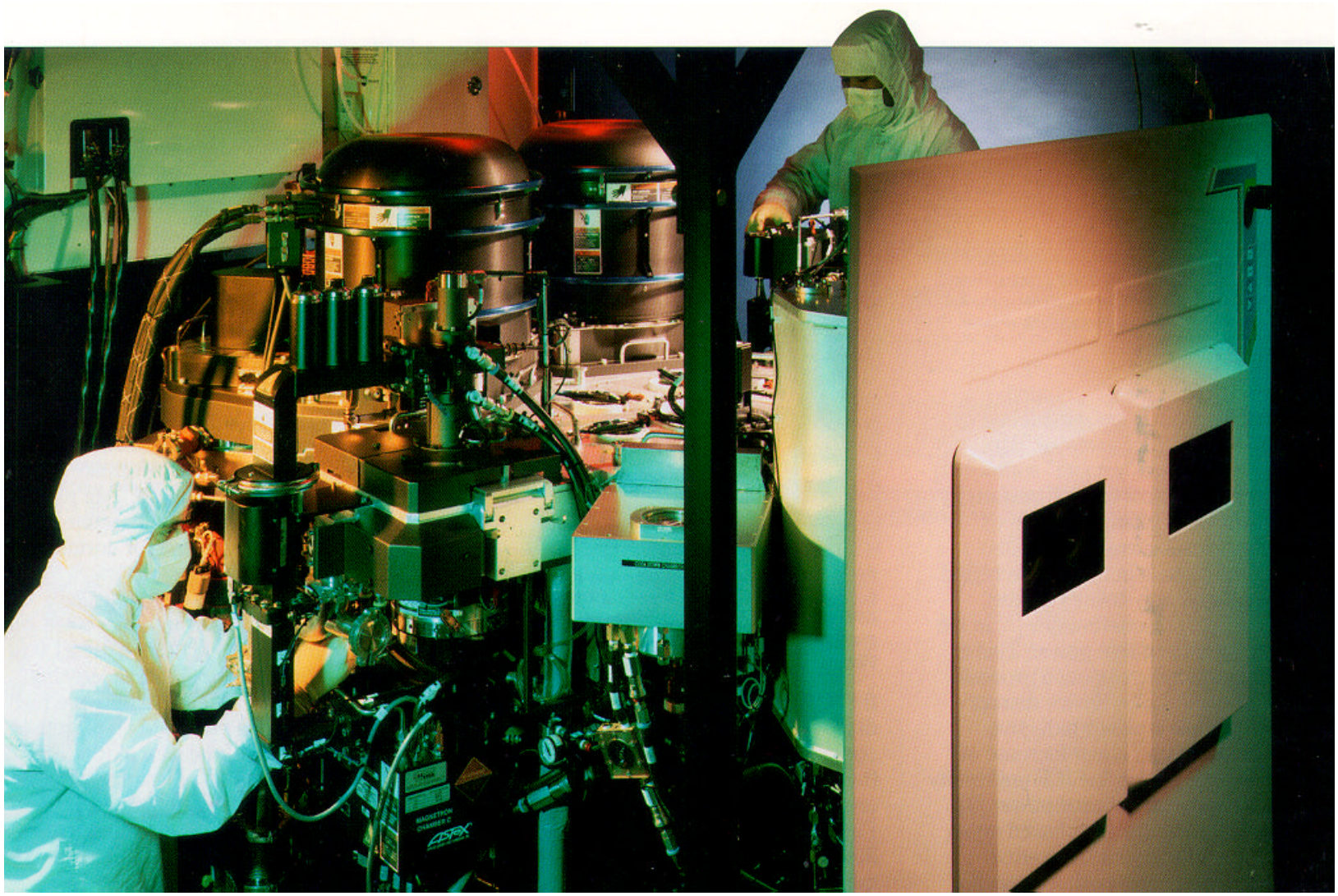


0.25 μm Feature (C. Cui, AMAT)

APPLIED MATERIALS DECOUPLED PLASMA SOURCE (DPS)



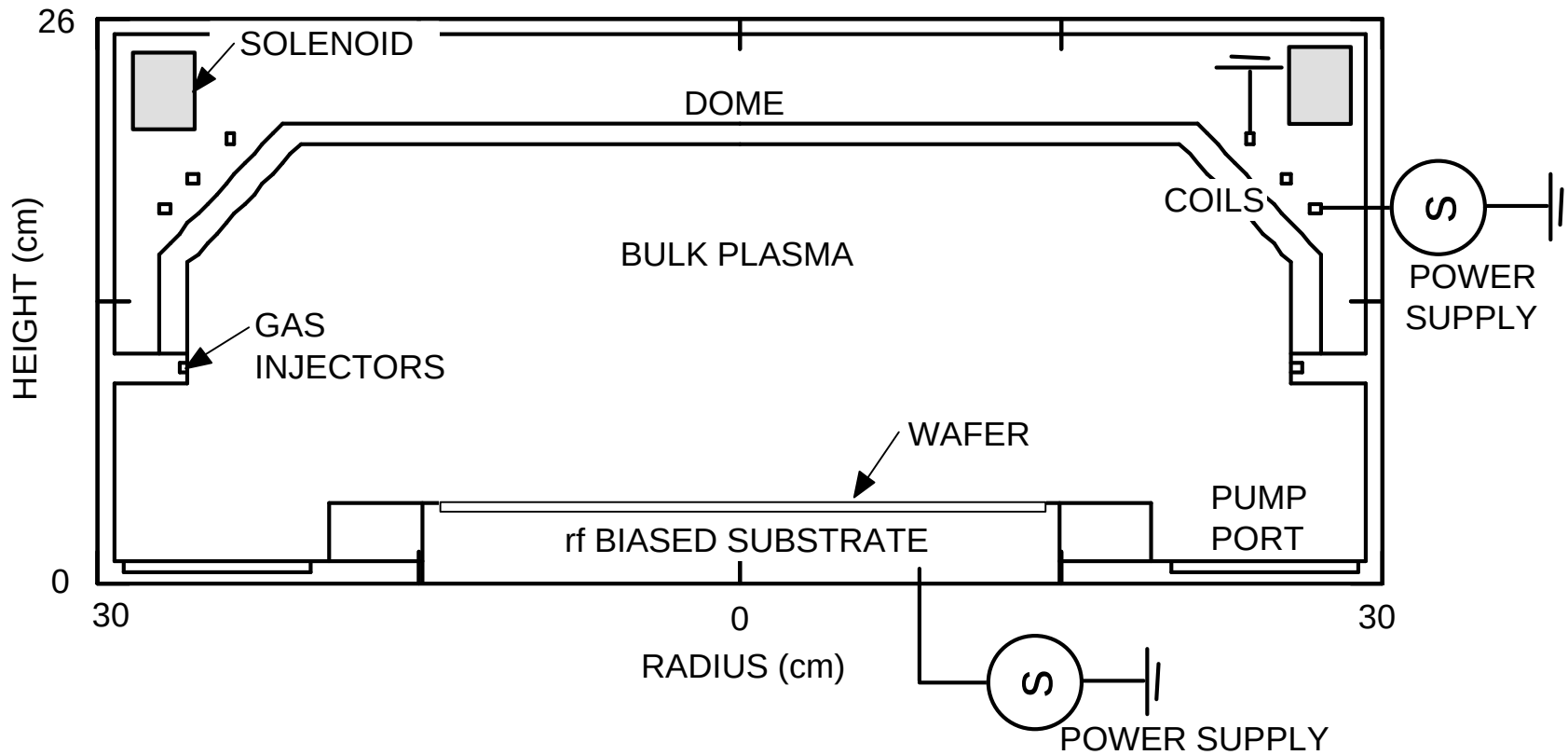
APPLIED MATERIALS DECOUPLED PLASMA SOURCE (DPS)



University of Illinois
Optical and Discharge Physics

TYPICAL PLASMA PROCESSING REACTOR

- **The typical low pressure (<10s - 100s mTorr) plasma processing reactor is powered by inductive and capacitive coupling, and may have auxiliary static magnetic fields.**



University of Illinois
Optical and Discharge Physics

WALK THROUGH: Ar/Cl_2 ICP TOOL

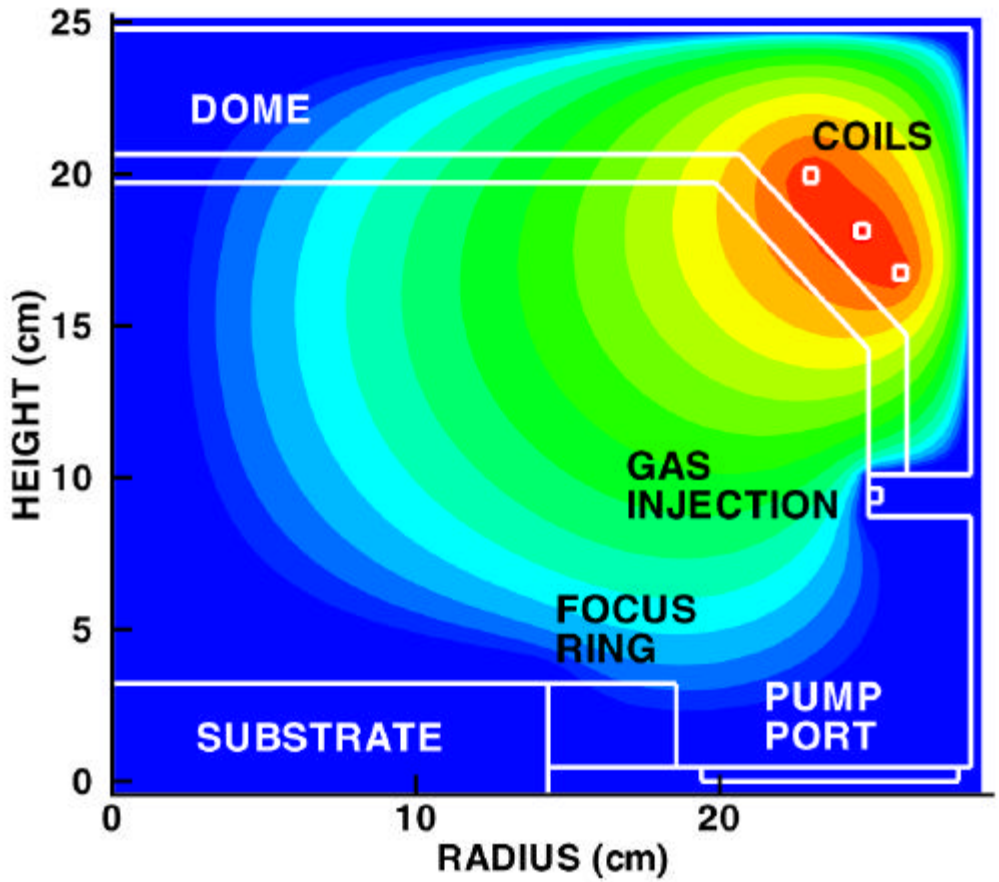
- **The general properties of an Ar/Cl_2 inductively coupled plasma tool will be examined.**

- **The inductively coupled electromagnetic fields have a skin depth of 3-4 cm.**

- **Absorption of the fields produces power deposition in the plasma.**

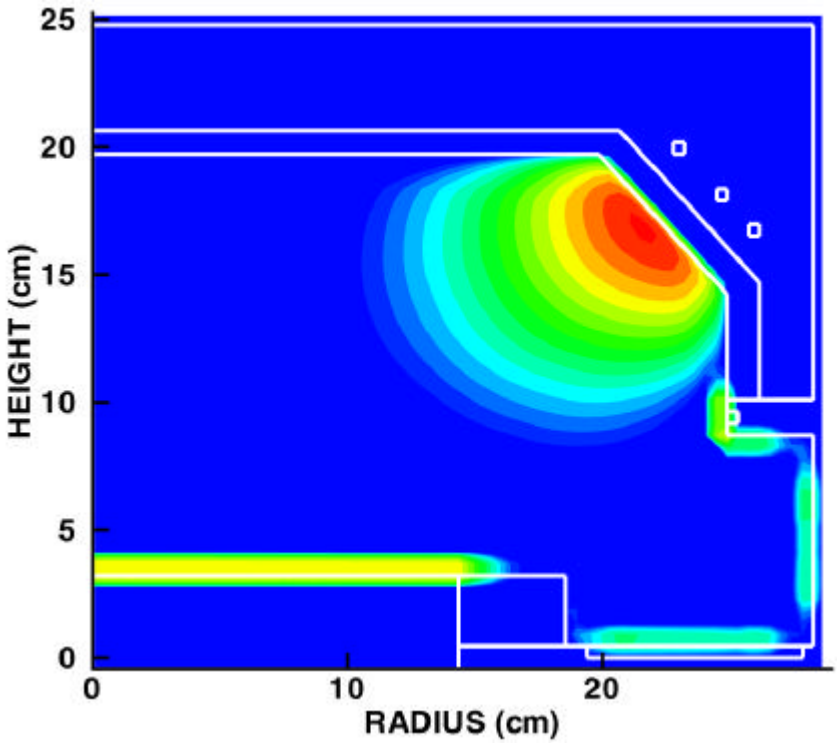
- **Electric Field (max = 6.3 V/cm)**

- **Ar/Cl_2 = 80/20**
- **20 mTorr**
- **1000 W ICP**
- **250 V bias, 2 MHz (260 W)**

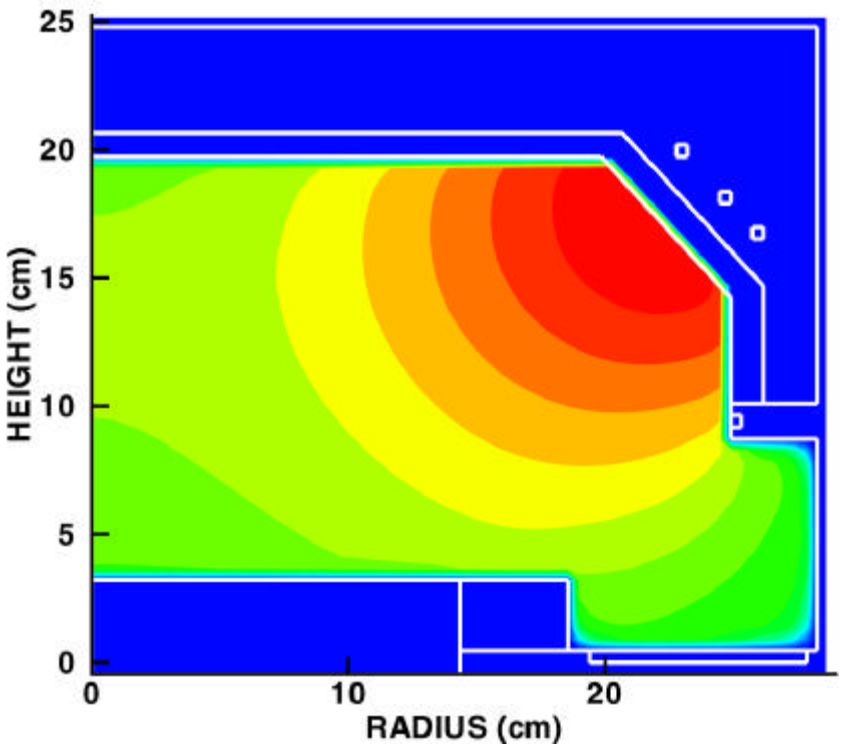


Ar/Cl_2 ICP TOOL: POWER AND ELECTRON TEMPERATURE

- **Power deposition from the inductive fields results in electron heating.**
- **At 2 MHz, power from the capacitive fields produces ion acceleration with little electron heating.**



Power Deposition (max = 0.91 W/cm^3)



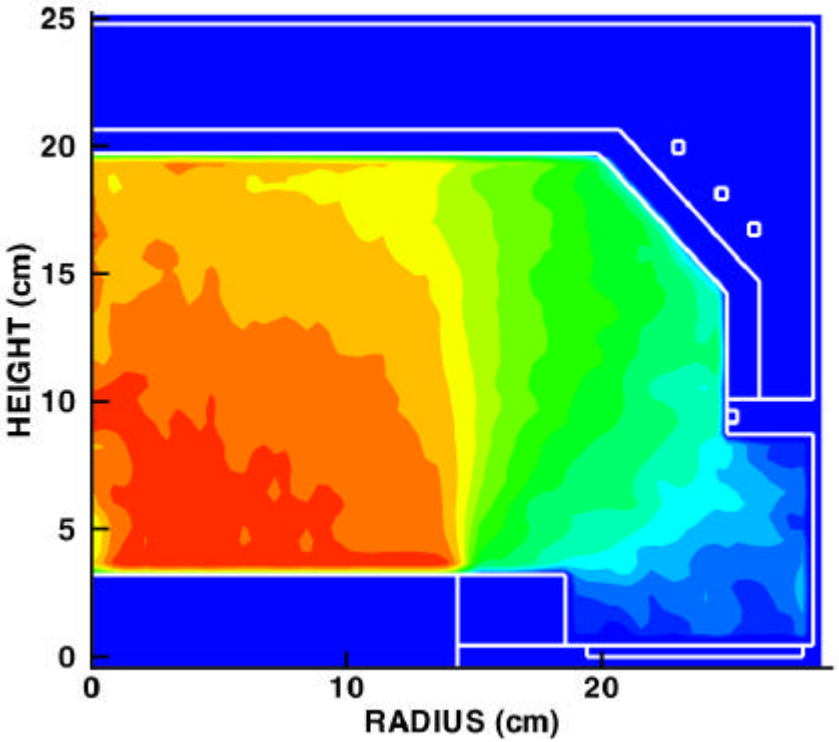
Electron Temperature (max = 5 eV)

- **Ar/Cl_2 = 80/20, 20 mTorr, 1000 W ICP, 250 V , 2 MHz bias (260 W)**

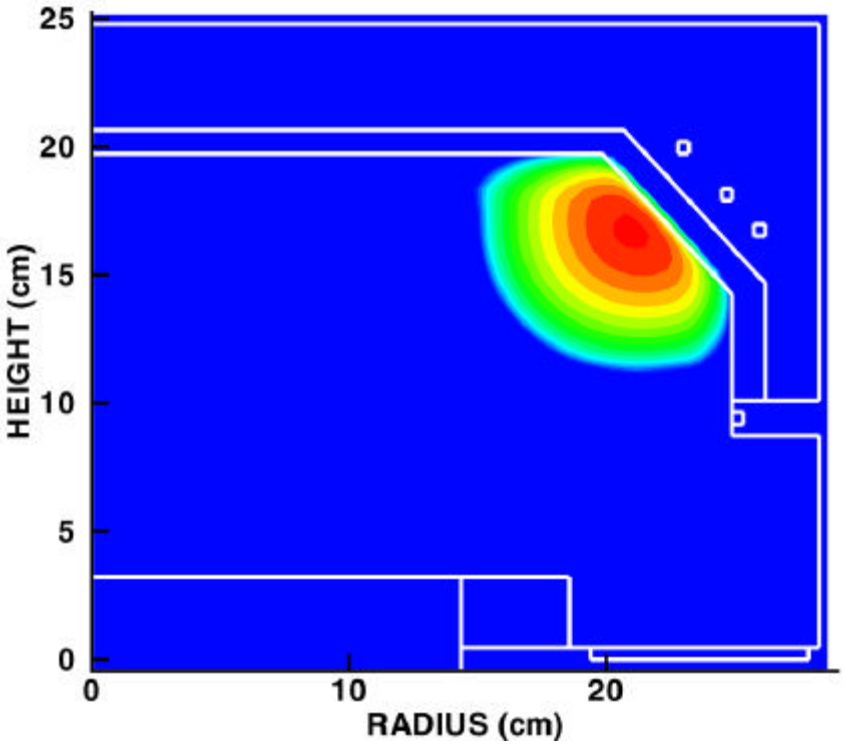
University of Illinois
Optical and Discharge Physics

Ar/Cl_2 ICP TOOL: IONIZATION

- **Electron impact ionization by the bulk electrons heated by the inductively coupled fields dominates.**
- **Ionization by sheath accelerated beam electrons is less important due to their long mean-free-paths at the low operating pressure.**



Beam ionization (max = 1.3 x 10^{14} /cm^3-s)

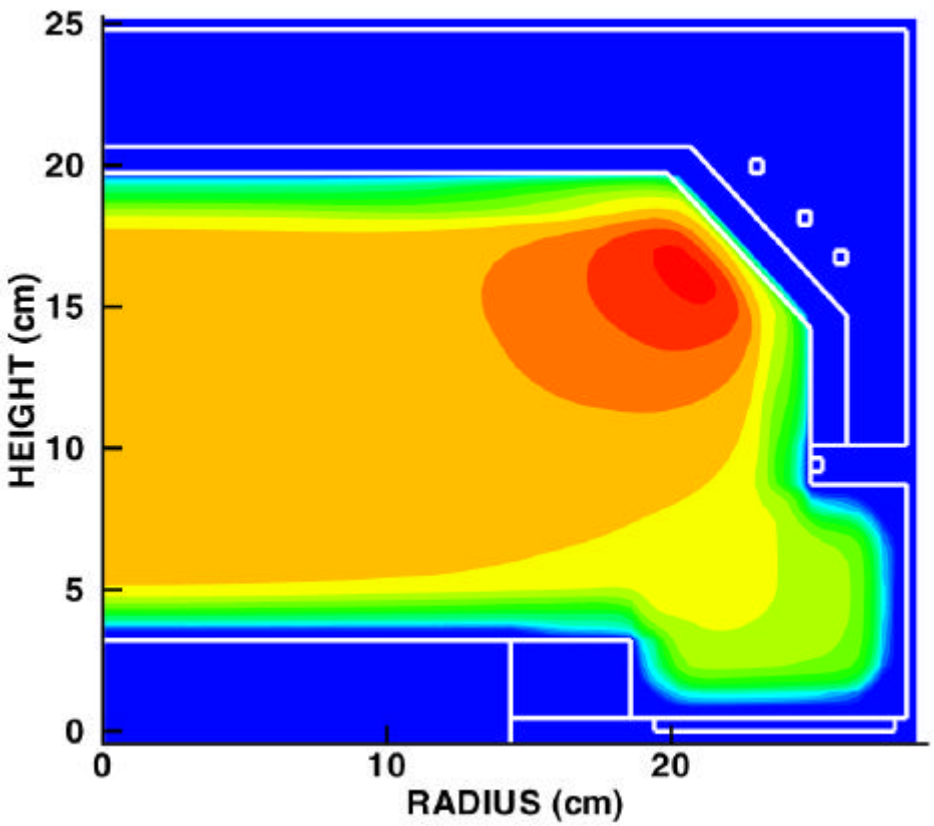


Bulk ionization (max = 5.4 x 10^{15} /cm^3-s)

- **Ar/Cl_2 = 80/20, 20 mTorr, 1000 W ICP, 250 V , 2 MHz bias (260 W)**

Ar/Cl_2 ICP TOOL: POSITIVE ION DENSITY

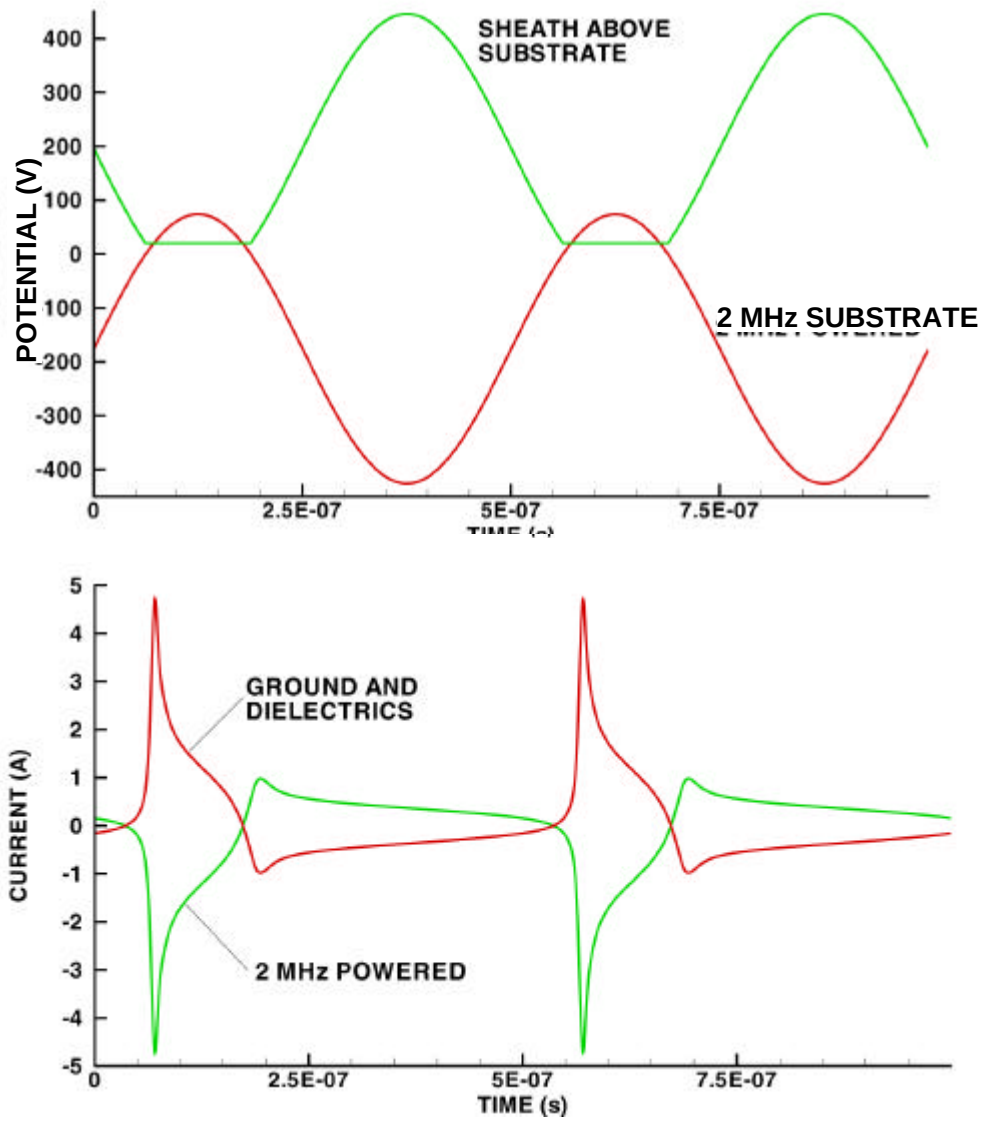
- **The diffusion of plasma from the remote sources produces a fairly uniform positive ion density in the vicinity of the substrate.**
- **In general, better uniformity is obtained with a bias than without.**



Positive Ion Density
(max = 1.8 x 10^{11} /cm^3-s)

- **Ar/Cl_2 = 80/20, 20 mTorr, 1000 W ICP, 250 V , 2 MHz bias (260 W)**

Ar/Cl_2 ICP TOOL: BIAS CURRENTS, POTENTIALS



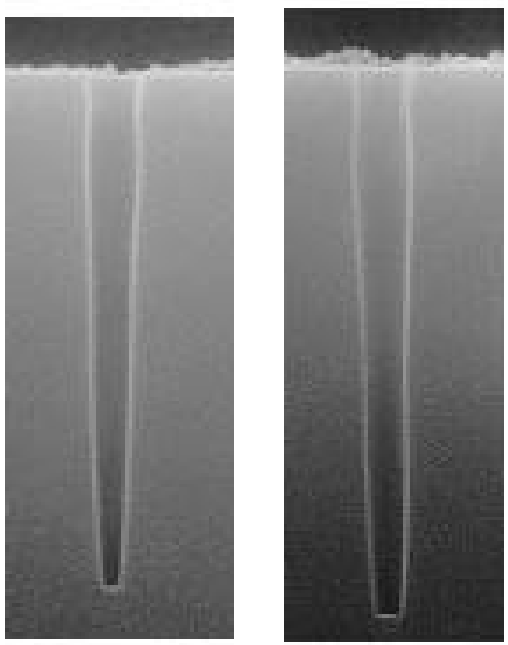
- **The small current collection area of the substract produces a large negative dc bias**
- **The large sheath potential results in electron current being collected during a small fraction of the rf cycle.**
- **The non-linearity of the sheaths at different surfaces also contributes to the non-sinusoidal current.**
- **Ar/Cl_2 = 80/20, 20 mTorr, 1000 W ICP, 250 V , 2 MHz bias (260 W)**

University of Illinois
Optical and Discharge Physics

INFLUENCE OF ION ENERGY ON ETCH PROFILE

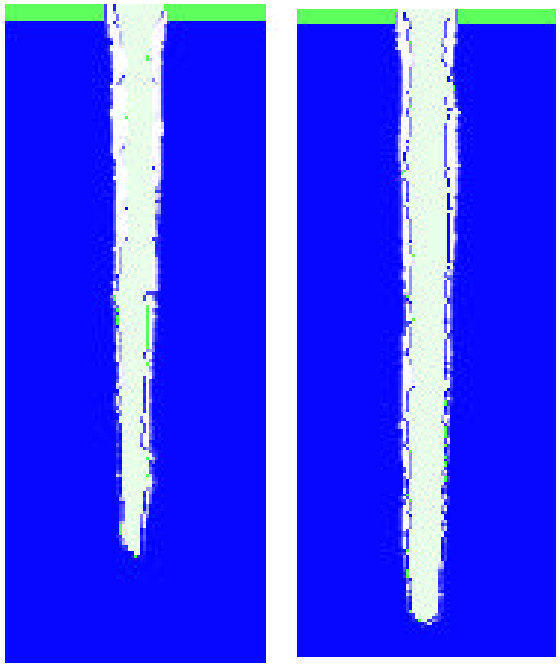
- **The acceleration of ions through the time varying sheaths produces directed fluxes to the substrates. The mixture of isotropic neutral radicals and anisotropic ions produces high aspect ratio etch profiles.**

EXPERIMENTS
(C. Cui, AMAT)



800 W 1000 W
BIAS POWER

SIMULATION



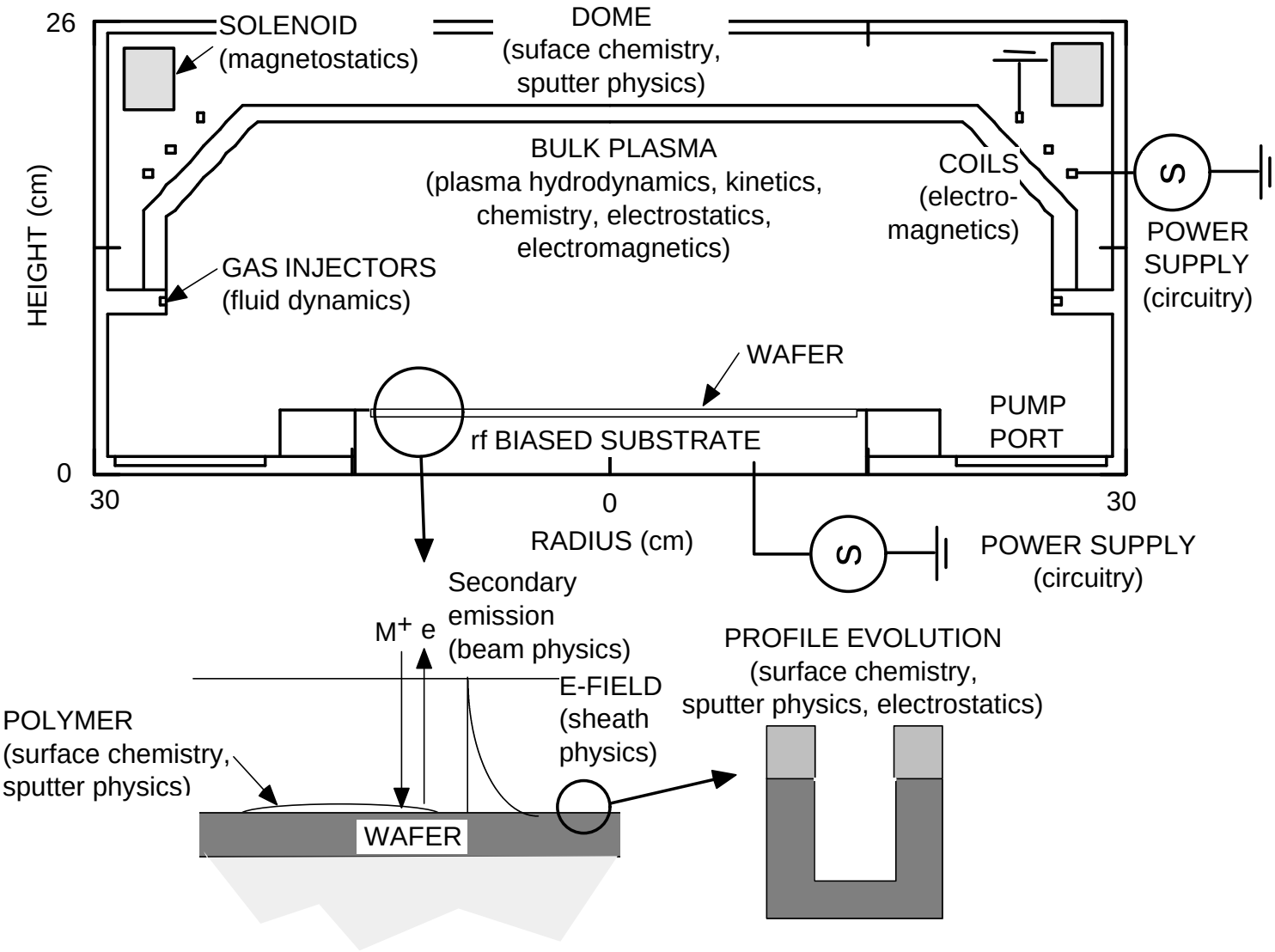
150 V 180 V
BIAS VOLTAGE

Example:

- **SiO_2 etching in an ICP fluorocarbon plasma with rf substrate bias.**

University of Illinois
Optical and Discharge Physics

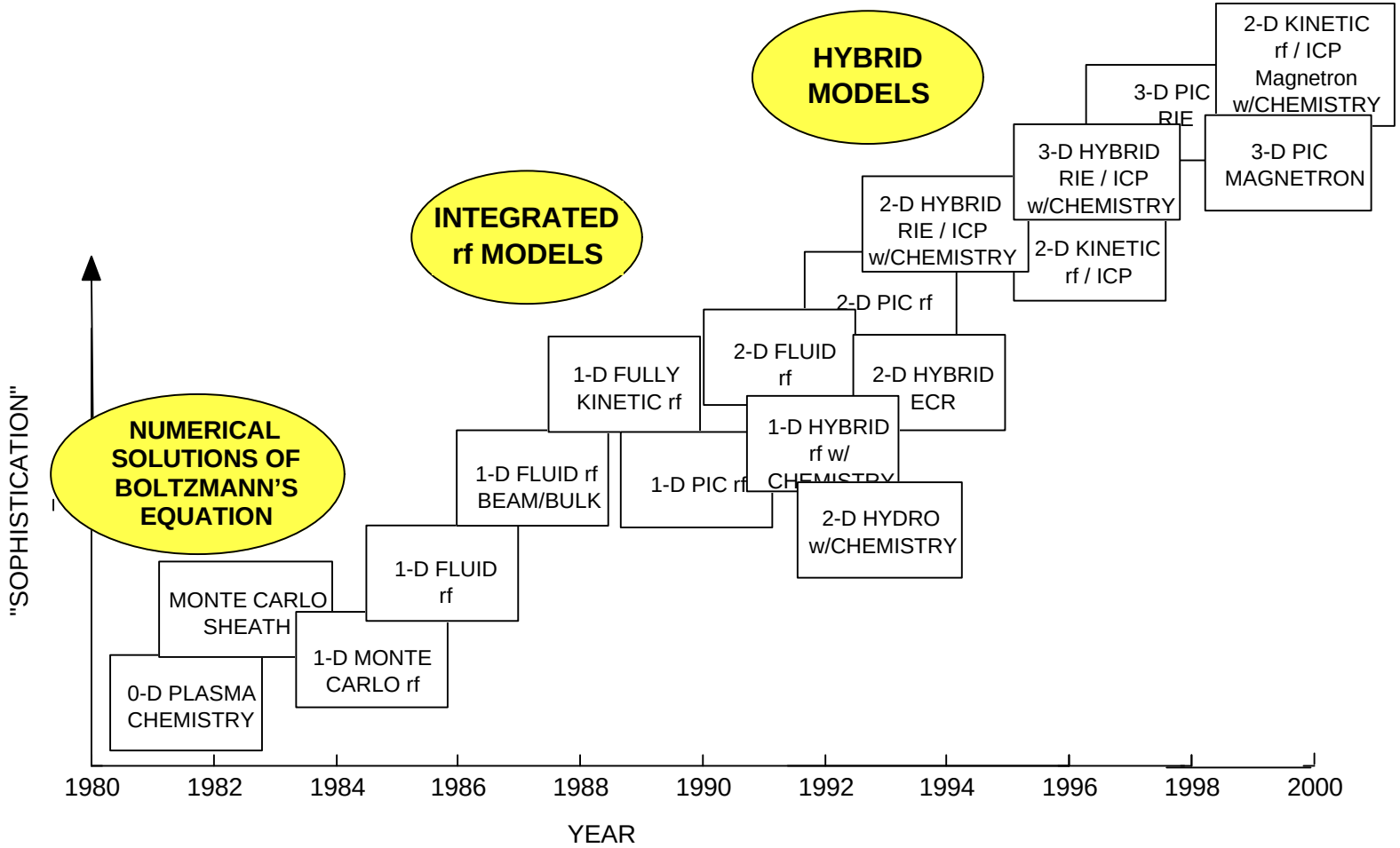
PHYSICS TO BE ADDRESSED



University of Illinois
Optical and Discharge Physics

IMPORTANT CONTRIBUTIONS TO MODELING INFRASTRUCTURE

- **The development of models for plasma processing has significantly progressed for almost 2 decades leveraging contributions from a wide range of disciplines.**



University of Illinois
Optical and Discharge Physics

MICROSCOPIC TO MACROSCOPIC: BOLTZMANN'S EQUATION

- **The coupling of atomic and molecular physics (i.e., atomic structure) to macroscopic properties (i.e., transport coefficients) is through moments of the electron energy distribution (EED) with collision cross sections.**

$$k = \int_0^\infty f(e)\left(\frac{2e}{m_e}\right)^{1/2} s(e)\,de$$

$f(e)$ **= Electron energy distribution**

$s(e)$ **= Electron collision cross section**

- **The EED is obtained through solution of the collisional Boltzmann's equation.**

$$\frac{\partial f(\vec{v})}{\partial t} = -\vec{v}\cdot\nabla_x \cdot f(\vec{v}) - \vec{a}\cdot\nabla_v f(\vec{v}) + \left(\frac{\partial f}{\partial t}\right)_c$$

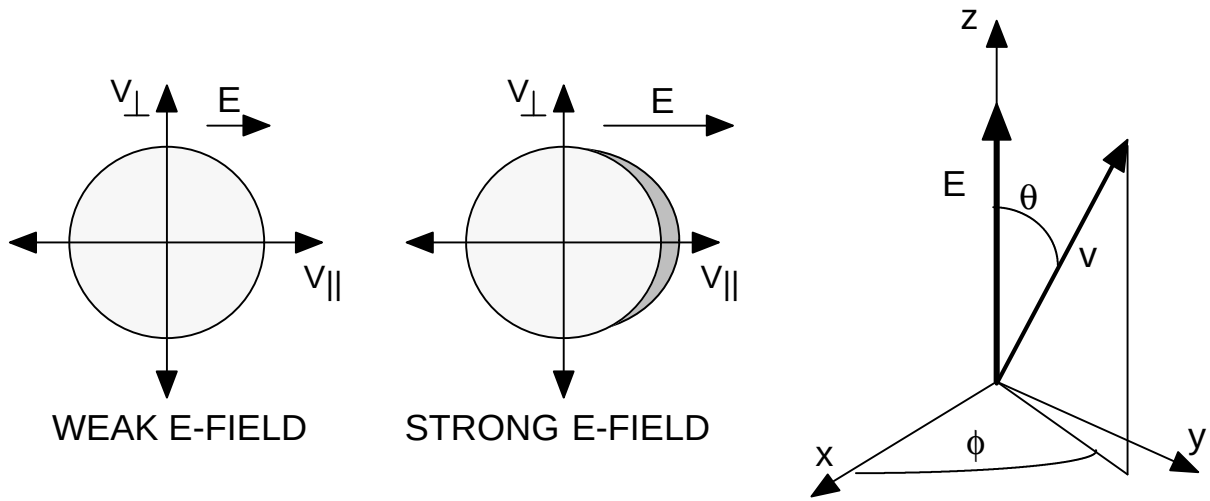
where the collision operator accounts for elastic, inelastic and super-elastic collsions.

- **The difficulty of solving BE with inelastic collisions stifled progress in modeling of complex plasma chemistries.**

University of Illinois
Optical and Discharge Physics

NUMERICAL SOLUTIONS OF BOLTZMANN'S EQUATION

- **In highly collisional plasmas with weak electric fields, the electron velocity distribution is essentially isotropic. As the field strengthens, $f(\vec{v})$ becomes only moderately anisotropic in the direction of the field.**



- **These conditions enabled the transformation of $f(\vec{v})$ to $f(|\vec{v}|)$ or $f(e)$ by using a spherical harmonic expansion about the angle between $\vec{v}$ and $\vec{E}$ (Allis, 1956; Shkarofsky, et al, 1966).**

$$f(\vec{v},\vec{r}) = \sum_i f_i(v,\vec{r}) P_i(q) =$$

$$f_o(v,\vec{r}) + f_1(v,\vec{r})\cos(q) + \ldots$$

f_o **= Isotropic component**

f_1 **= Anisotropic component**

NUMERICAL SOLUTIONS OF BOLTZMANN'S EQUATION

- **With the advent of high speed computers, this formulation was numerically implemented with increasing sophistication to address science and technological issues.**

W. L. Nighan (PRA, 2, 1989 (1970)	**EEDs in molecular gases for electric discharge lasers**
S. D. Rockwood (PRA 8, 2348 (1973))	**Electron-electron collisions**
L. Pitchford and A. Phelps (PRA 1980-1990)	**Higher order expansions to address higher degrees of anisotropy; density gradient expansions**
C. M. Ferreira; M. Capitelli and C. Gorse (1985-1995)	**Coupling of EED with excitation of internal modes of molecules**
W. L. Morgan (CPC 58, 127 (1990))	**ELENDIF (first publically available collisional Boltzmann solver)**

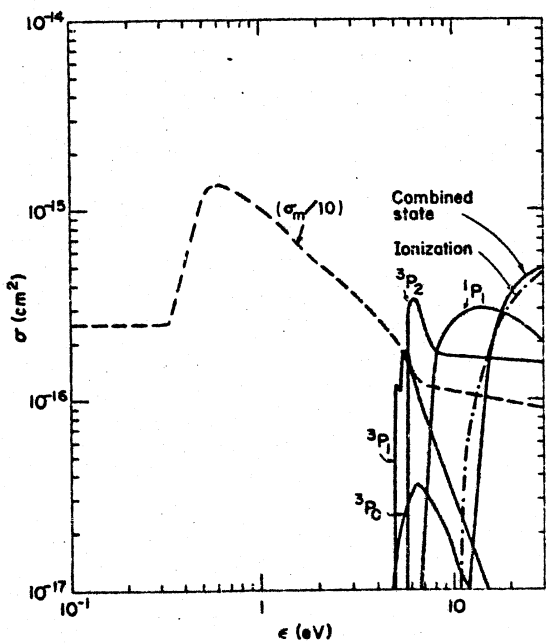
- **A flurry of activity in the 1980s resulted in a fundamental understanding of the dynammics of EEDs in collisional plasmas, which produced a core knowledge for present modeling activities.**

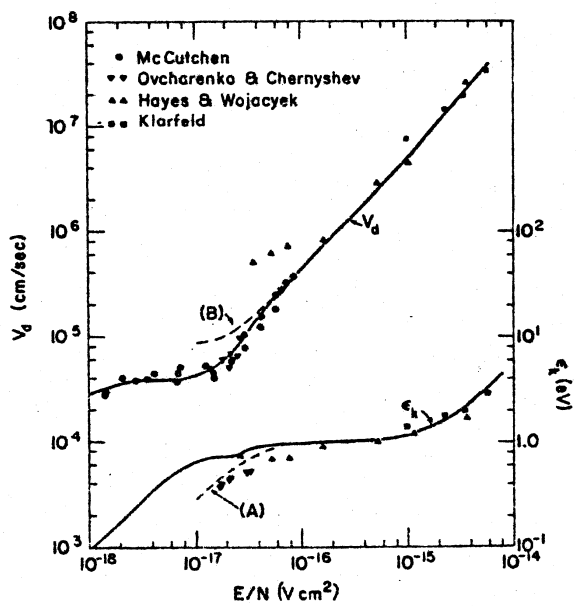
ELECTRON IMPACT CROSS SECTIONS FROM SWARM DATA

- **Rockwood's work stands out for "standardizing" numerical solutions of Boltzmann's equation including inelastic and electron-electron collisions.**
- **The method borrows from Allis, and Canavan and Proctor in the use of fluxes of electrons along the energy axis in phase space.**

$$\frac{\partial n}{\partial t} = -\frac{\partial J_f}{\partial \epsilon} - \frac{\partial J_{cl}}{\partial \epsilon} + \sum_{s,j} N_s^0 \Big(R_{sj}(\epsilon+\epsilon_{sj}^*)\, n(\epsilon+\epsilon_{sj}^*) + R'_{sj}(\epsilon-\epsilon_{sj}^*)\, n(\epsilon-\epsilon_{sj}^*)\, N_s^j/N_s^0$$

$$+ R_s^i(\epsilon+\epsilon_{si}^*)\, n(\epsilon+\epsilon_{si}^*) + \delta(\epsilon)\int_{\epsilon_{si}^*}^{\infty} R_s^i(\epsilon)\, n(\epsilon)\, d\epsilon - [R_{sj}(\epsilon) + R'_{sj}(\epsilon) + R_s^i(\epsilon)]\, n(\epsilon)\Big).$$





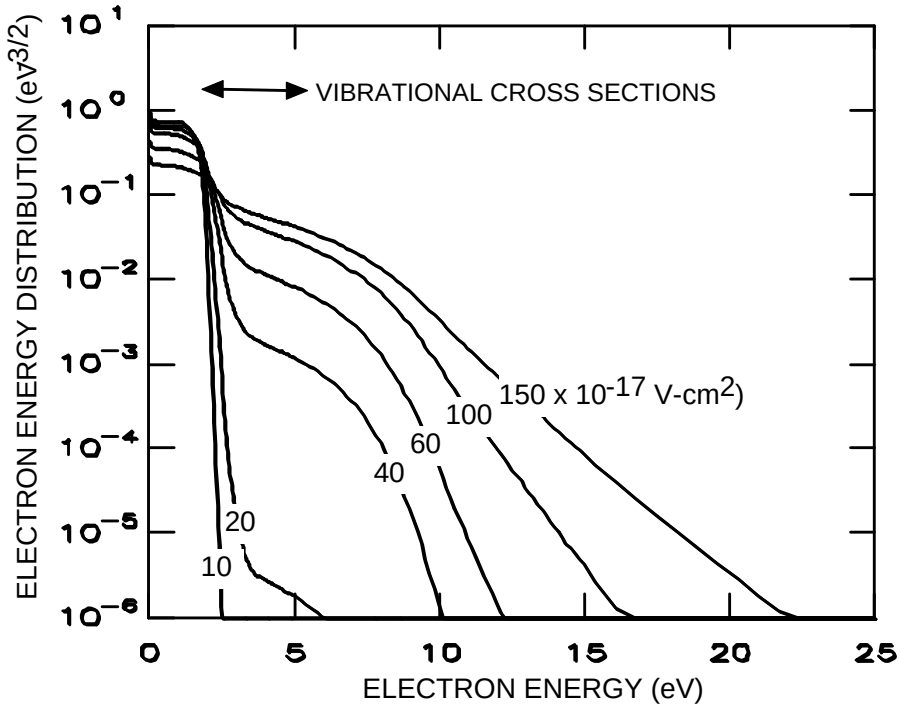
- **Rockwood demonstrated the method by "backing out" electron impact cross sections from swarm data for Hg, values still in use today.**
- **PRA 8, 2348 (1973)**

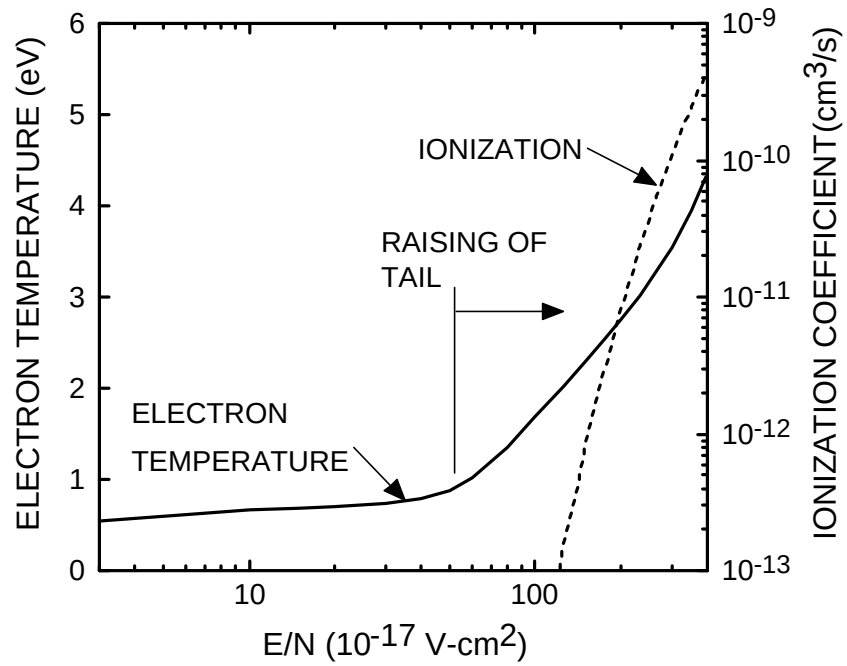
University of Illinois
Optical and Discharge Physics

ELECTRON SWARM PROPERTIES: N_2

- **The availability of "Commodity" numerical solutions of Boltzmann's equation enabled fundamental properties of electron interactions with molecules to be accurately incorporated into plasma equipment models.**

- **Example: Electron swarm properties in N_2: The low energy vibrational cross sections produce a "cut-off" EED whose tail rises only at high E/N.**

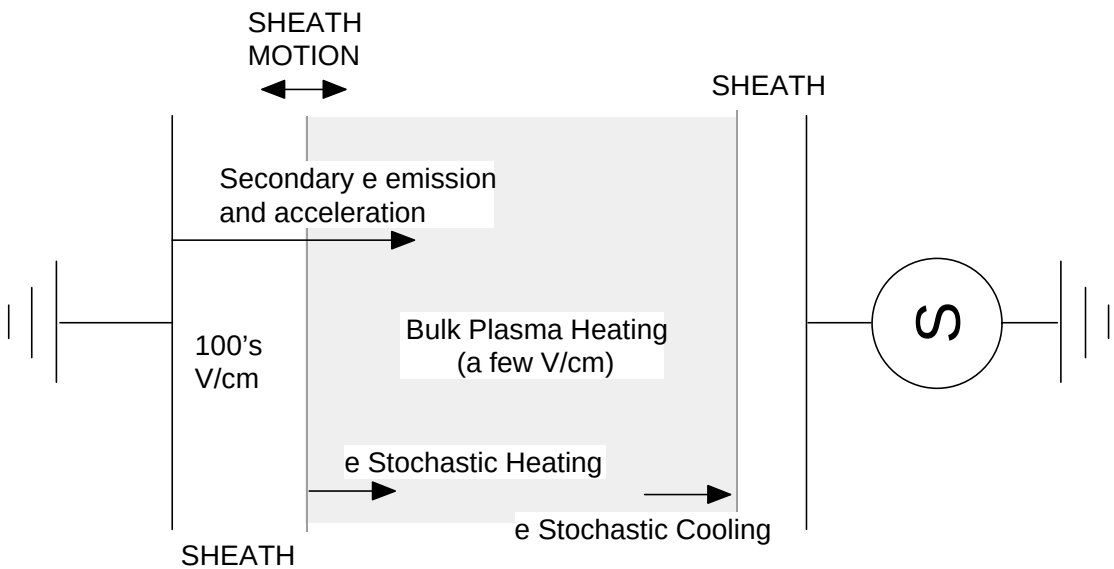




University of Illinois
Optical and Discharge Physics

INTEGRATED PLASMA MODELS: RF DISCHARGES

- **The fundamental understanding of electron swarms afforded by mastery of Boltzmann's equation enabled integrated plasma models to evolve.**
- **Integrated models are time and spatially dependent accountings of electron, ion and neutral transport while including consequences of "chemistry" and "boundaries".**
- **The first integrated models were for capacitively coupled rf discharges in which sheath motion produces electron heating.**



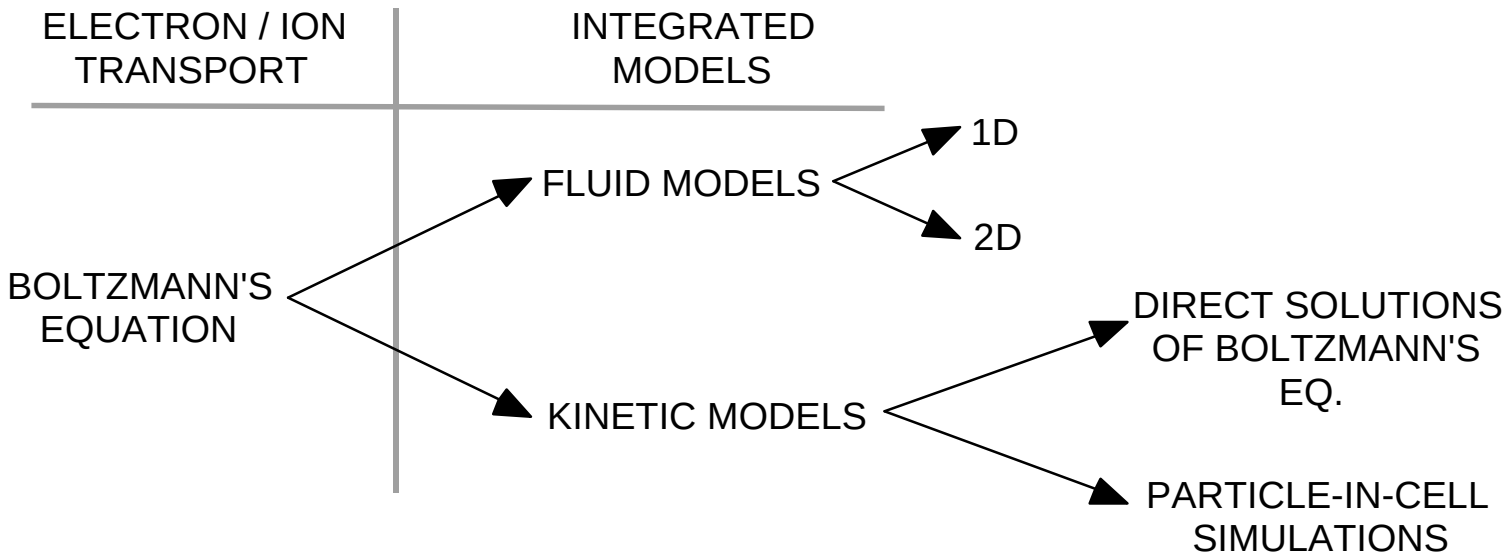
End Results:

- **Potentials**
- **EEDs**
- **Heating and excitation rates**
- **Energy resolved ion fluxes to substrate**

University of Illinois
Optical and Discharge Physics

METHODOLOGIES FOR INTEGRATED MODELS

- **Given the baseline fundamental understanding of electron transport afforded by mastery of Boltzmann's equation, 2 methodologies evolved for integrated plasma models:**

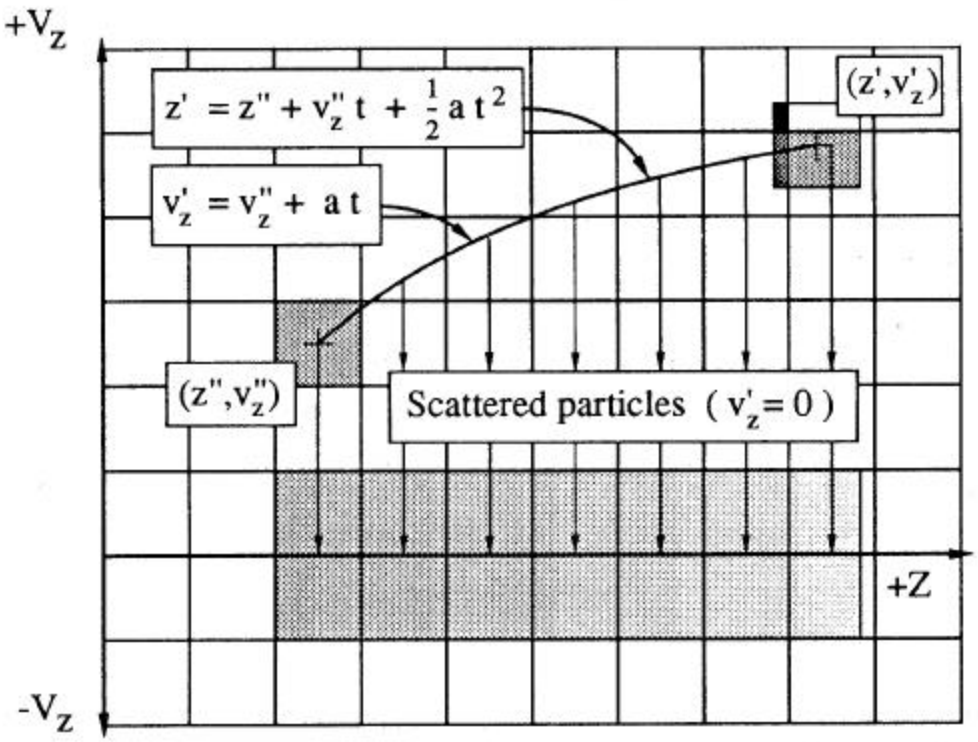


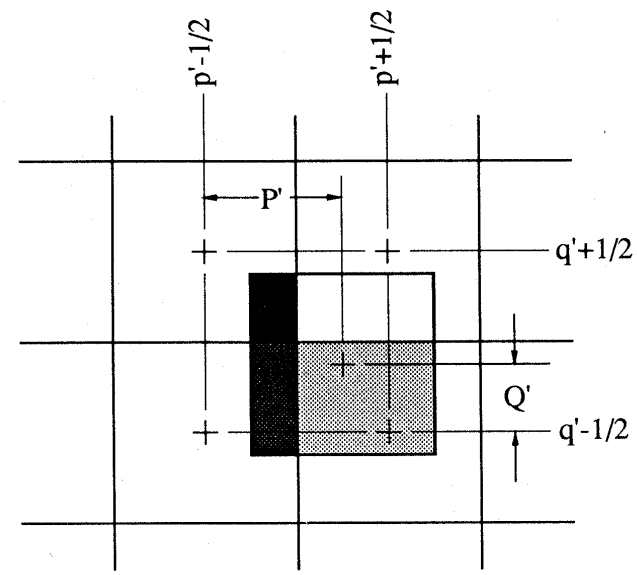
- **Kinetic models are time and spatially dependent solutions of Boltzmann's equation which produce electron and ion velocity distributions, either directly or statistically.**

- **Fluid models solve moments of Boltzmann's equation.**

DIRECTION INTEGRATION OF BOLTZMANN'S EQUATION

- **Although computationally intensive, integrating Boltzmann's equation for $f(\vec{v},\vec{r},t)$ provides the most detail and is least dependent on apriori assumptions.**
- **Direct integrations typically involved use of "propagators" or Greens functions to transport electron and ion pseudoparticles through the $(\vec{v},\vec{r})$ phase space.**

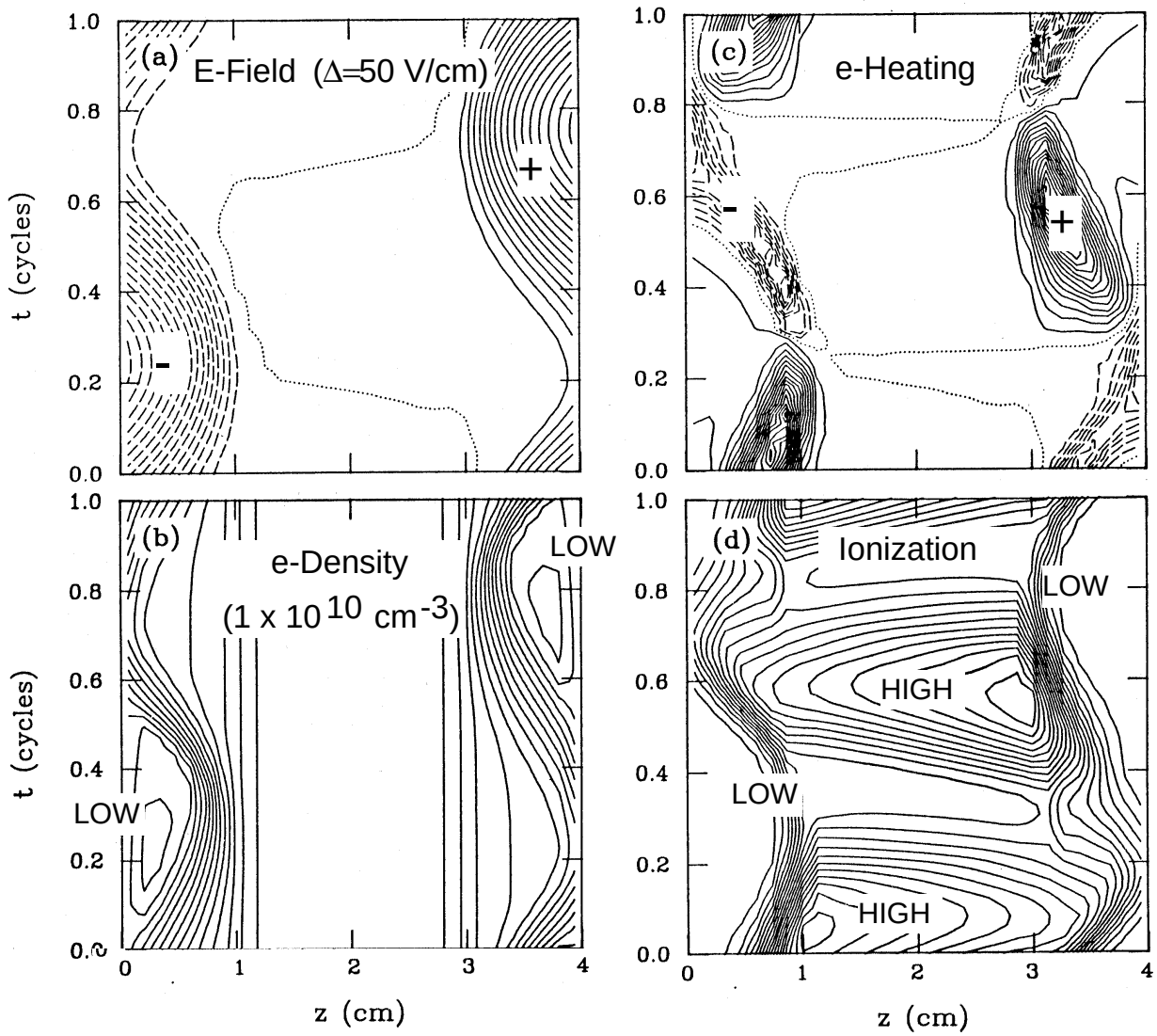




T. J. Sommerer, et. al., PRA 43, 4452 (1991)

University of Illinois
Optical and Discharge Physics

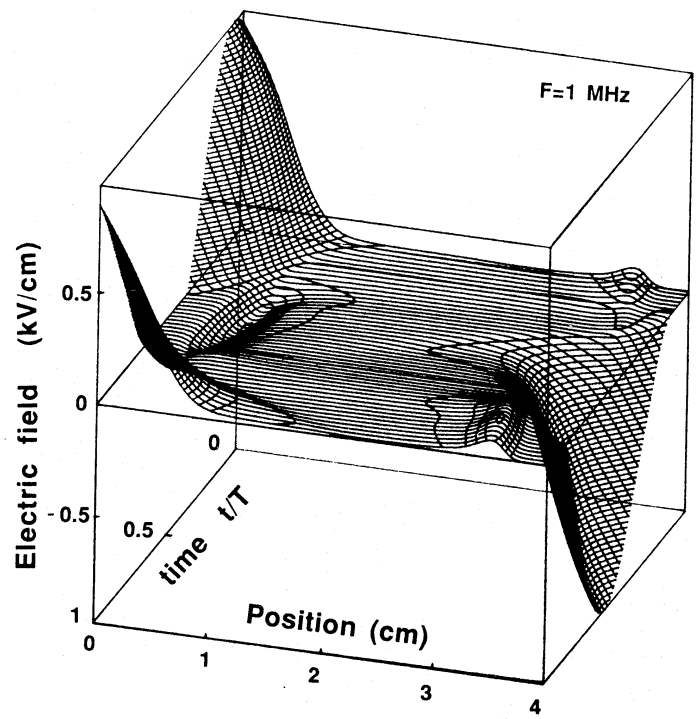
RF DISCHARGE IN He: STOCHASTIC HEATING

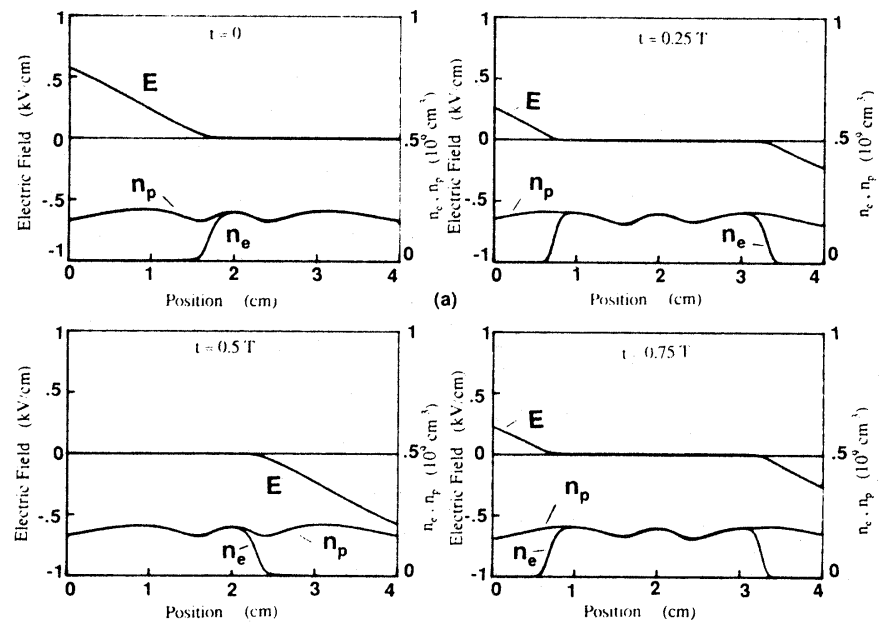


- **Solving BE using a Greens function or "propagator" method, Sommerer et al (PRA 43, 4452 (1991)) demonstrates stochastic heating.**
- **He, 13.56 MHz, 0.1 Torr, 500 V**

FLUID MODELING OF rf DISCHARGES: 1D

- **Early fluid modeling of rf discharges were 1-d simulations using simple gases and "local" electron momentum and energy transport.**
- **Large strides were made in our understanding of both discharge dynamics and numerical methods.**





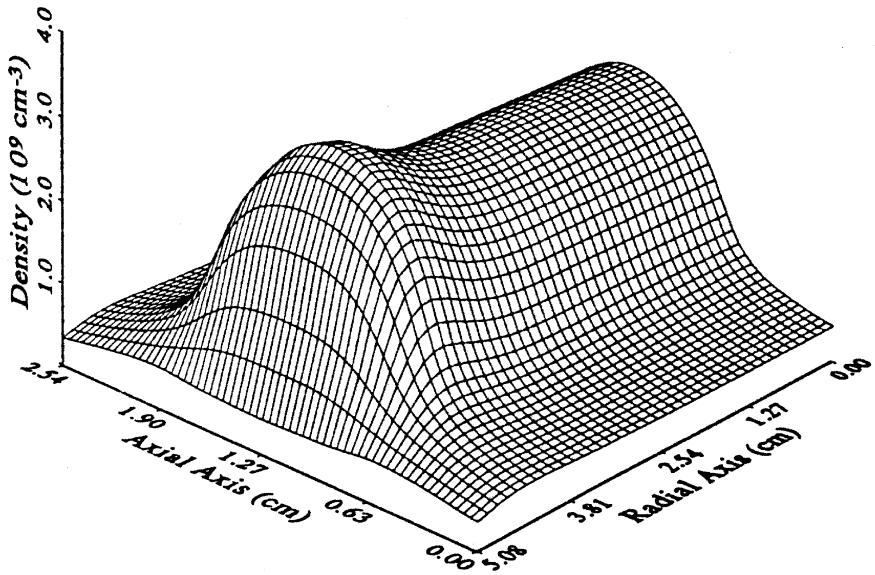
He/electronegative gas, 1 MHz, 1 Torr

- **J. P. Bouef, Phys. Rev. A 36, 2782 (1987)**

University of Illinois
Optical and Discharge Physics

FLUID MODELING OF rf DISCHARGES: 2D

- **Increasing sophistication in numerical methods and availability of computing power allowed higher dimensionality and more complete physics in fluid modeling.**
- **Fully hydrodynamic 2-d models demonstrated "edge effects" in rf discharges which still dominate design considerations of etch tools.**



$$\frac{\partial n_e}{\partial t} = -\nabla \cdot (u_e n_e) + u n_e$$

$$\frac{\partial (m n_e u_e)}{\partial t} = -\nabla \cdot (m n_e u_e u_e) - n_e q E - \nabla P_e - \frac{m n_e u_e}{\tau_m}$$

$$\frac{\partial n_e w}{\partial t} = -\nabla \cdot (n_e w u_e) - n_e q u_e E - \nabla \cdot (u_e P_e) - \frac{n_e w}{\tau_w}.$$

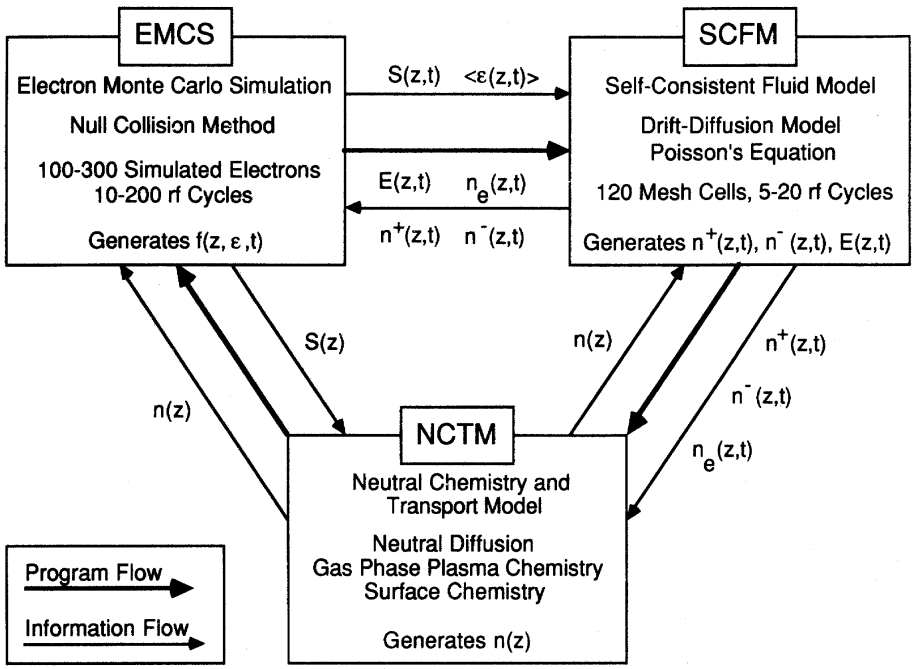
- **He, 13.56 MHz, 1 Torr**

- **F. F. Young and C-H. Wu, Trans. Plasma Sci. 21, 312 (1992)**

University of Illinois
Optical and Discharge Physics

HYBRID MODELING OF rf DISCHARGES

- As chemistries became more complex, the need for kinetically derived transport coefficients and rate constants increased.
- Since fluid methods have significant computational advantages over purely kinetic formulations, hybrid models evolved to meet these needs.

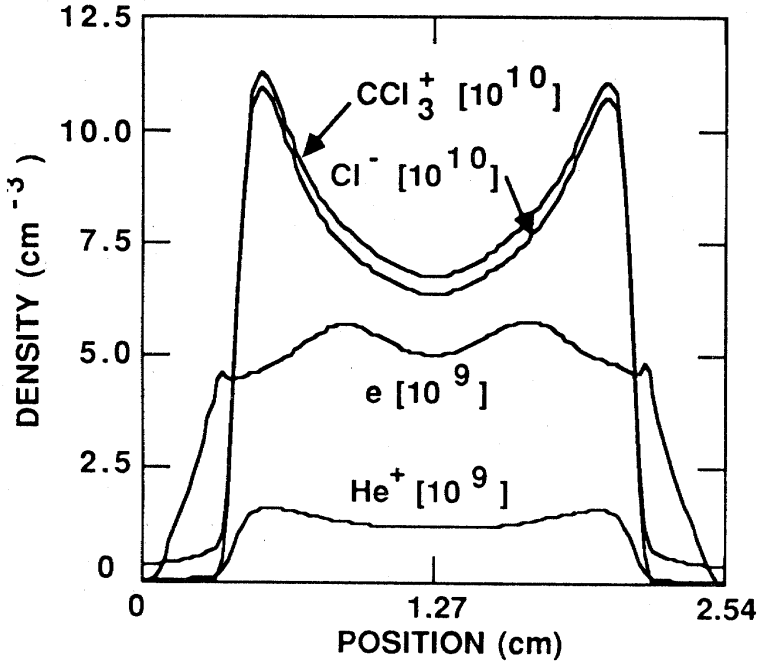


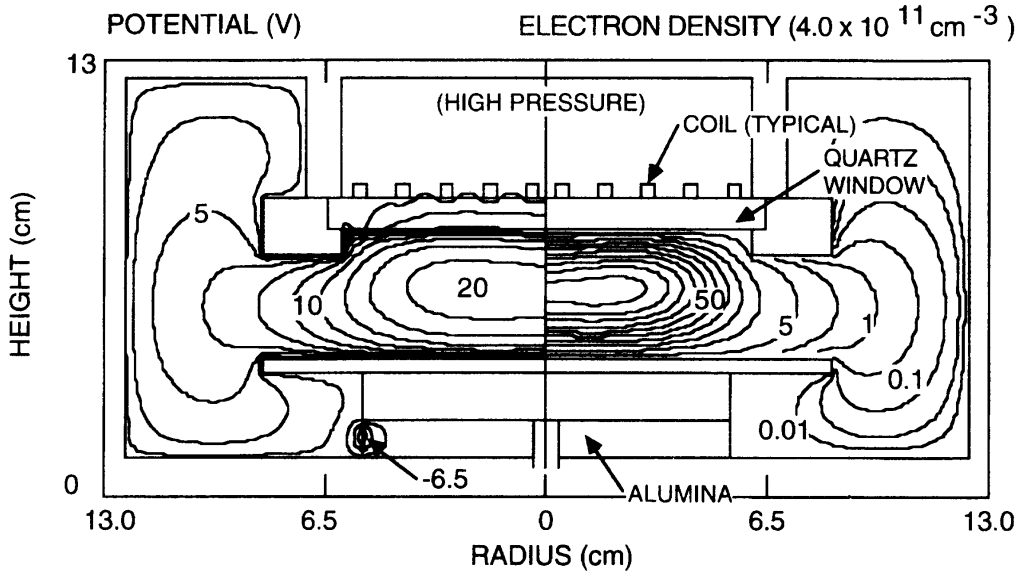
- In hybrid models, different numerical techniques are iteratively combined to address different physics or different time/spatial scales.
- Kinetic methods are used for non-local energy transport to derive transport coefficients.
- Fluid methods provide densities and electric fields.
- Sommerer and Kushner, J. Appl. Phys. 71, 1654 (1992)

University of Illinois
Optical and Discharge Physics

HYBRID MODELING OF rf DISCHARGES

- **Hybrid techniques enabled complex gas chemistries to be addressed and, with including additional modules, modeling of electromagnetically excited systems, such as inductively coupled plasmas (ICPs).**



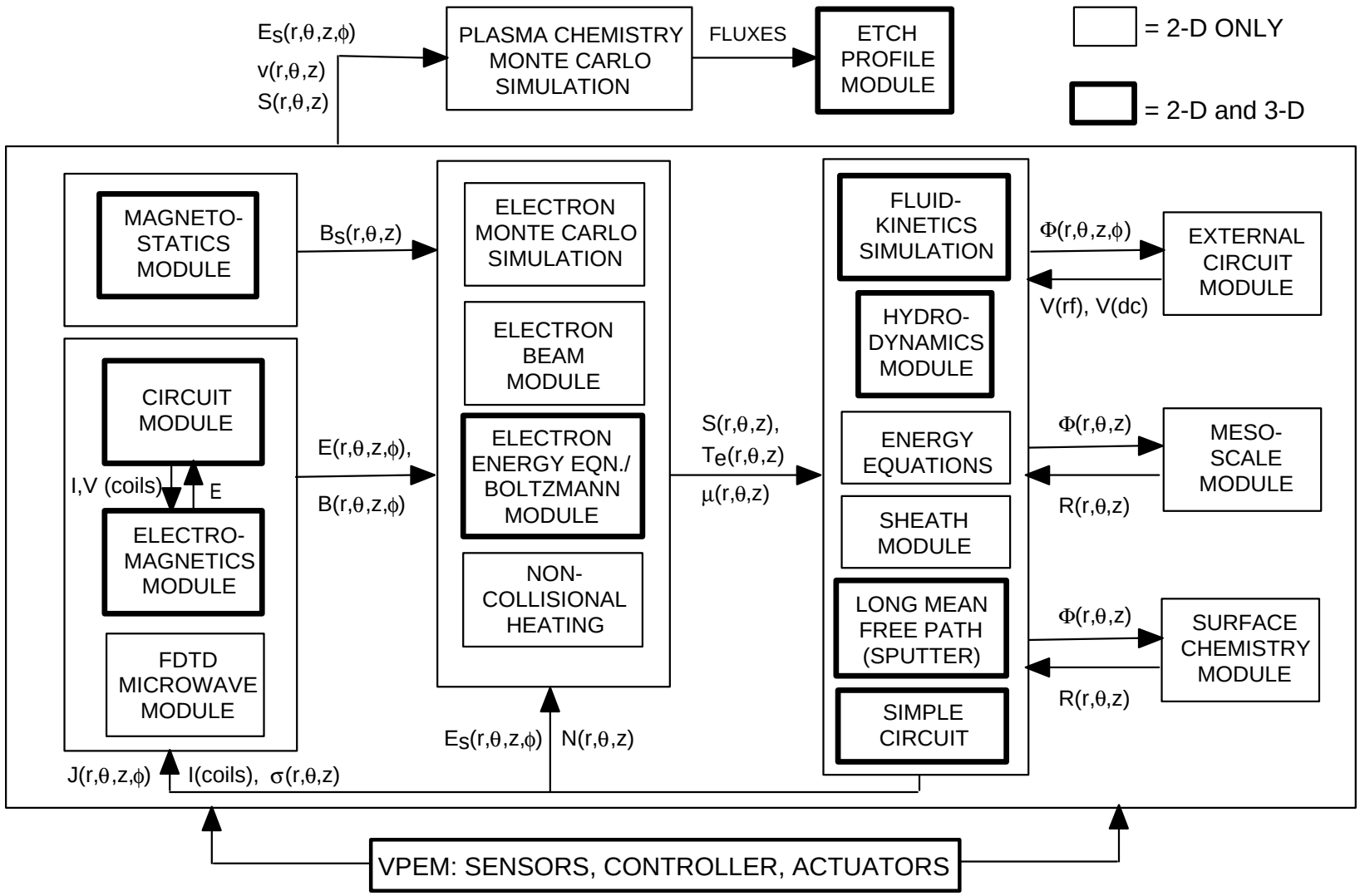


- **He/CCl_4=9/1, 0.25 Torr, 600 V**
- **Sommerer et al, JVST B 10, 2179 (1992)**

- **Ar, 10 mTorr, 150 W**
- **Ventzek et al. JVST B 12, 3118 (1994)**

University of Illinois
Optical and Discharge Physics

SCHEMATIC OF THE HYBRID PLASMA EQUIPMENT MODEL



University of Illinois
Optical and Discharge Physics

PEUG9904

ELECTROMAGNETICS

- **The wave equation is typically solved in the frequency domain:**

$$-\nabla\left(\frac{1}{m}\nabla\cdot\overline{E}\right)+\nabla\cdot\left(\frac{1}{m}\nabla\overline{E}\right)=\frac{\partial^2\left(e\overline{E}\right)}{\partial t^2}+\frac{\partial\left(s\overline{E}+\overline{J}\right)}{\partial t}$$

$$s=\sum_{\mathrm{j}}\frac{\mathrm{q}^2\mathrm{n}_{\mathrm{j}}}{\mathrm{m}_{\mathrm{j}}n_{\mathrm{j}}\left(1-\frac{\mathrm{i}w}{n_{\mathrm{j}}}\right)}$$

$$\vec{\mathrm{E}}(\vec{\mathrm{r}},\mathrm{t})=\vec{\mathrm{E}}'(\vec{\mathrm{r}})exp(-\mathrm{i}(w\mathrm{t}+j(\vec{\mathrm{r}})))$$

- **With static applied magnetic fields, conductivities are tensor quantities:**

$$\ddot{s}=s_{\mathrm{o}}\frac{\mathrm{m}n_{\mathrm{m}}}{\mathrm{q}a}\frac{1}{\left(a^2+\left|\vec{\mathrm{B}}\right|^2\right)}\begin{pmatrix} a^2+\mathrm{B}_{\mathrm{r}}^2 & a\mathrm{B}_{\mathrm{z}}+\mathrm{B}_{\mathrm{r}}\mathrm{B}_q & -a\mathrm{B}_q+\mathrm{B}_{\mathrm{r}}\mathrm{B}_{\mathrm{z}} \\ -a\mathrm{B}_{\mathrm{z}}+\mathrm{B}_{\mathrm{r}}\mathrm{B}_q & a^2+\mathrm{B}_q^2 & a\mathrm{B}_{\mathrm{r}}+\mathrm{B}_q\mathrm{B}_{\mathrm{z}} \\ -a\mathrm{B}_q+\mathrm{B}_{\mathrm{r}}\mathrm{B}_{\mathrm{z}} & -a\mathrm{B}_{\mathrm{r}}+\mathrm{B}_q\mathrm{B}_{\mathrm{z}} & a^2+\mathrm{B}_{\mathrm{z}}^2 \end{pmatrix}$$

$$\vec{\mathrm{j}}=\ddot{s}\cdot\vec{\mathrm{E}} \qquad a=\frac{(\mathrm{i}w+n_{\mathrm{m}})}{\mathrm{q}/\mathrm{m}},\quad s_{\mathrm{o}}=\frac{\mathrm{q}^2\mathrm{n}_{\mathrm{e}}}{\mathrm{m}n_{\mathrm{m}}}$$

- **Circuit models are used to provide antenna currents.**

University of Illinois
Optical and Discharge Physics

ELECTRON ENERGY TRANSPORT

- **Under conditions where collisional heating and diffusive transport dominate, electron transport coefficients and electron impact source functions are obtained by solving the electron energy equation.**

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

where

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

- **Transport coefficients are obtained as a function of average energy (ε = (2/3) T_e) from solution of Boltzmann' Equation for the electron energy distribution.**

University of Illinois
Optical and Discharge Physics

ELECTRON ENERGY TRANSPORT

- **When electron energy deposition is non-collisional and/or transport is non-diffusional, Monte Carlo techniques are used.**
  - **Secondary electron emission and acceleration through sheaths.**
  - **Wave heating and trapping.**
  - **Long mean-free-path transport.**

- **Conduction currents are kinetically derived from the MCS for use in solving the wave equation.**

$$\mathbf{J}_e(\mathbf{r}) = J_0(\mathbf{r}) \exp(i\phi_V(\mathbf{r}))\, \hat{\theta} = -q\, n_e(\mathbf{r})\, v_\theta(\mathbf{r}) \exp(i\phi_V(\mathbf{r}))\, \hat{\theta}\,.$$

University of Illinois
Optical and Discharge Physics

PLASMA CHEMISTRY, TRANSPORT AND ELECTROSTATICS

- **Multi-fluid techniques are used where continuity, momentum and energy equations are solved for each species, with coupling terms for exchange of momentum and energy.**

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

$$\frac{\partial (N_i \vec{v}_i)}{\partial t} = \frac{1}{m_i} \nabla (k N_i T_i) - \nabla \cdot (N_i \vec{v}_i \vec{v}_i) + \frac{q_i N_i}{m_i} \left(\vec{E} + \vec{v}_i \times \vec{B}\right) - \nabla \cdot \overline{m}_i$$

$$- \sum_j \frac{m_j}{m_i + m_j} N_i N_j \left(\vec{v}_i - \vec{v}_j\right) \nu_{ij}$$

$$\frac{\partial (N_i e_i)}{\partial t} + \nabla \cdot Q_i + P_i \nabla \cdot U_i + \nabla \cdot (N_i U_i e_i) = \frac{N_i q_i^2 \nu_i}{m_i (\nu_i^2 + w^2)} E^2$$

$$+ \frac{N_i q_i^2}{m_i \nu_i} E_s^2 + \sum_j 3 \frac{m_{ij}}{m_i + m_j} N_i N_j R_{ij} k_B (T_j - T_i) \pm \sum_j 3 N_i N_j R_{ij} k_B T_j \quad ,$$

- **Slip boundary conditions are used for neutral transport for momentum and energy to address momentum and temperature jump conditions.**

PLASMA CHEMISTRY, TRANSPORT AND ELECTROSTATICS

- **Given the hierarchy of time scales and large number of species, fully implicit solutions of all transport equations are typically not done.**

- **Due to the extremely short dielectric relaxation times (< 10^{-12} s), Poisson's equation must be implicitly solved.**

- **A typical method uses a prediction of densities for the time at which the fields will be used. Surface charges are included here.**

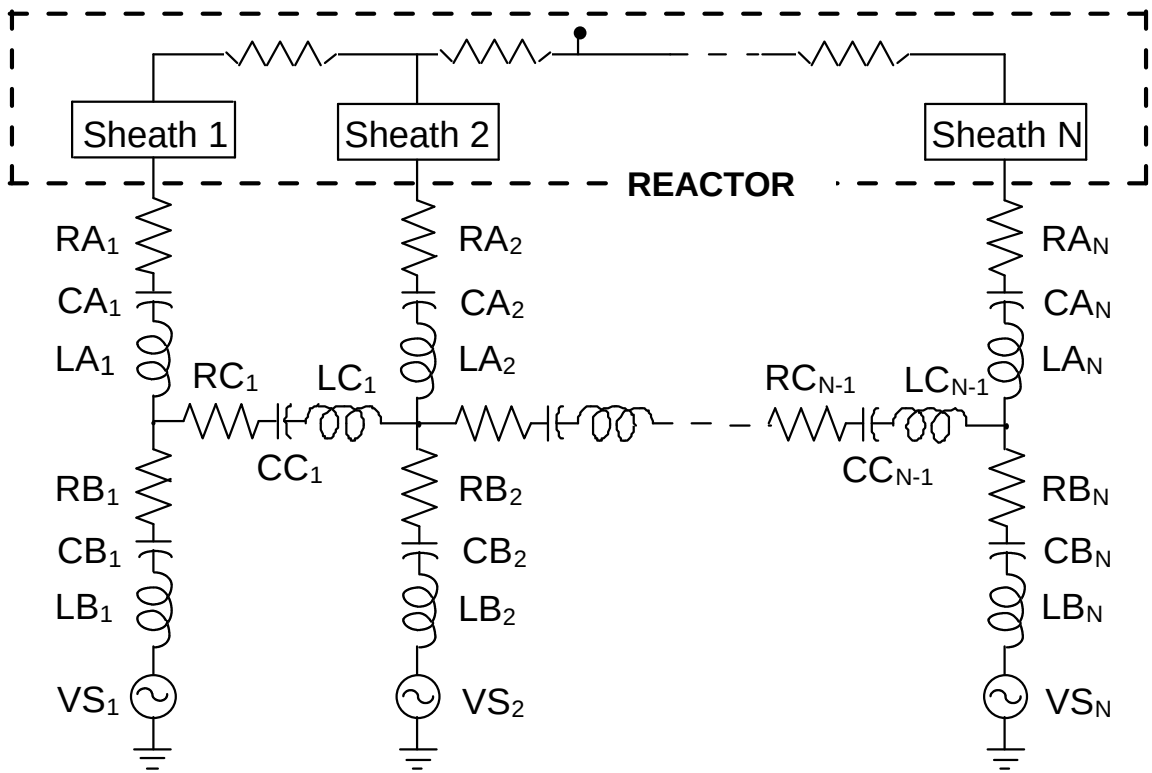
$$\nabla \cdot e \nabla \Phi(t + \Delta t) = -\left(r_s + \sum_i q_i N_i - \Delta t \cdot \sum_i \left(q_i \nabla \cdot \vec{f}_i \right) \right)$$

- **When sheaths are not resolved by the mesh, semi-analytic models are used to obtain sheath potentials, which are inserted as potential "jump-conditions" at surfaces.**

University of Illinois
Optical and Discharge Physics

CIRCUIT MODELS

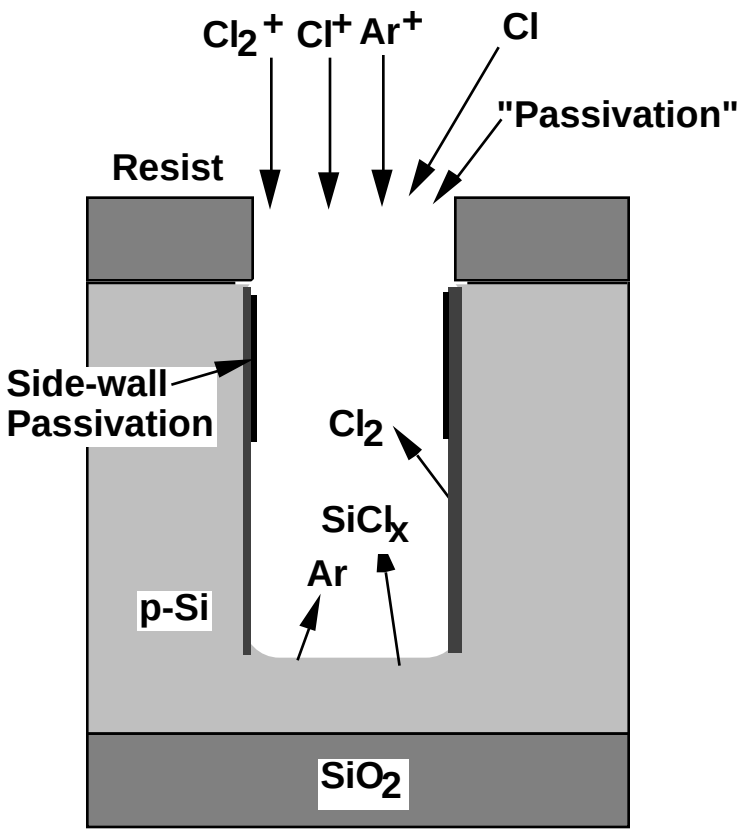
- **Circuit models for the reactor and driving electronics provide voltage harmonics (amplitude and phase) on metal surfaces for solution of Poisson's equation.**



- **Sheath models are typically employed to account for non-linearities in the plasma response to harmonic excitation.**

University of Illinois
Optical and Discharge Physics

MONTE CARLO FEATURE PROFILE MODEL (MCFP)



- The MCFP model predicts time and spatially dependent etch profiles using neutral and ion fluxes from the PCMCS.
- Any chemical mechanism may be implemented in the MCFP using a "plasma chemistry" input hierarchy.

  e.g., $Cl^+ + SiCl_2(s) > SiCl_2(g)$

- All pertinent processes can be included: thermal etch, ion assisted etch, sputter, redeposition, passivation.
- Energy dependent etch processes may be implemented using parametric forms.
- The MCFP may utilize ALL flux statistics from the PCMCS
  - Ion energy and angular distributions
  - Neutral energy and angular distributions
  - Position dependent fluxes

EXAMPLES OF PLASMA EQUIPMENT MODELING FOR TOOL DESIGN

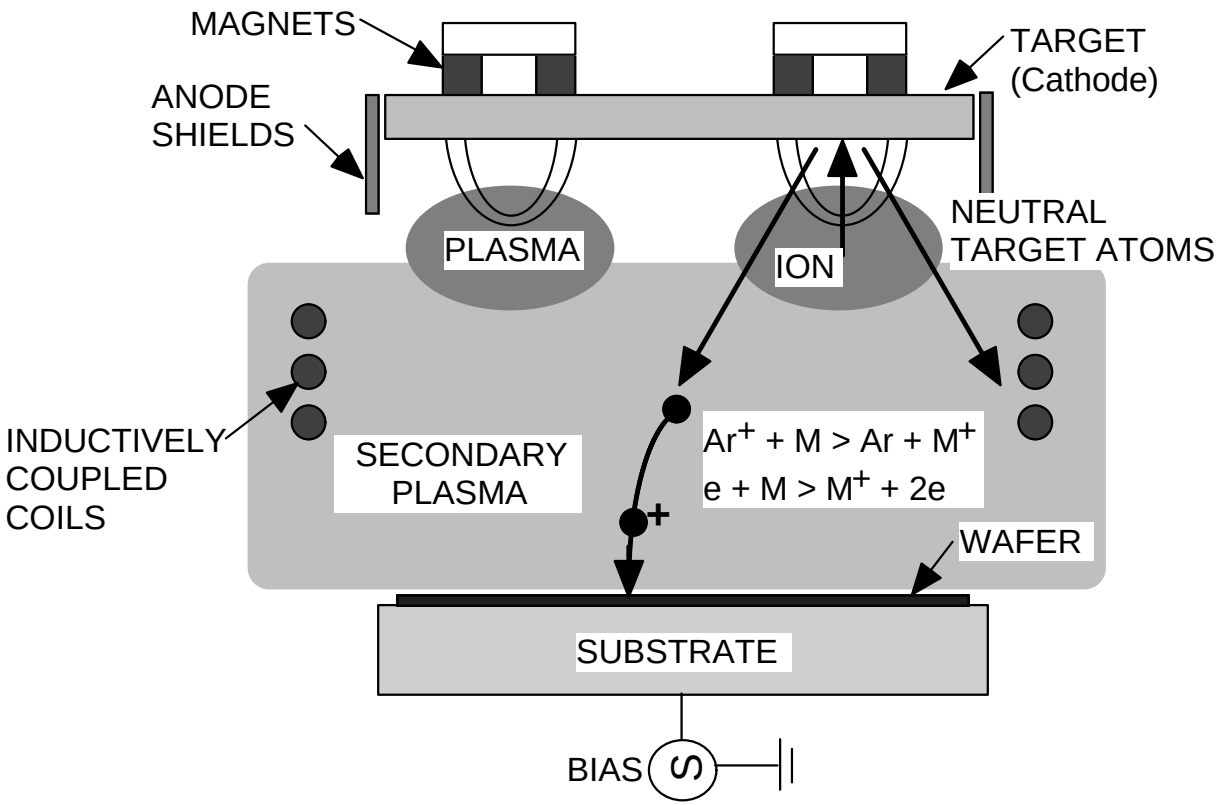
IONIZED METAL PHYSICAL VAPOR DEPOSITION

MAGNETICALLY ENHANCED INDUCTIVELY COUPLED PLASMAS

University of Illinois
Optical and Discharge Physics

IONIZED METAL PHYSICAL VAPOR DEPOSITION

- **Ionized Metal PVD (IMPVD) is being developed to fill deep vias and trenches for interconnect, and for deposition of seed layers and diffusion barriers.**
- **In IMPVD, a second plasma source is used to ionize a large fraction of the sputtered metal atoms prior to reaching the substrate.**



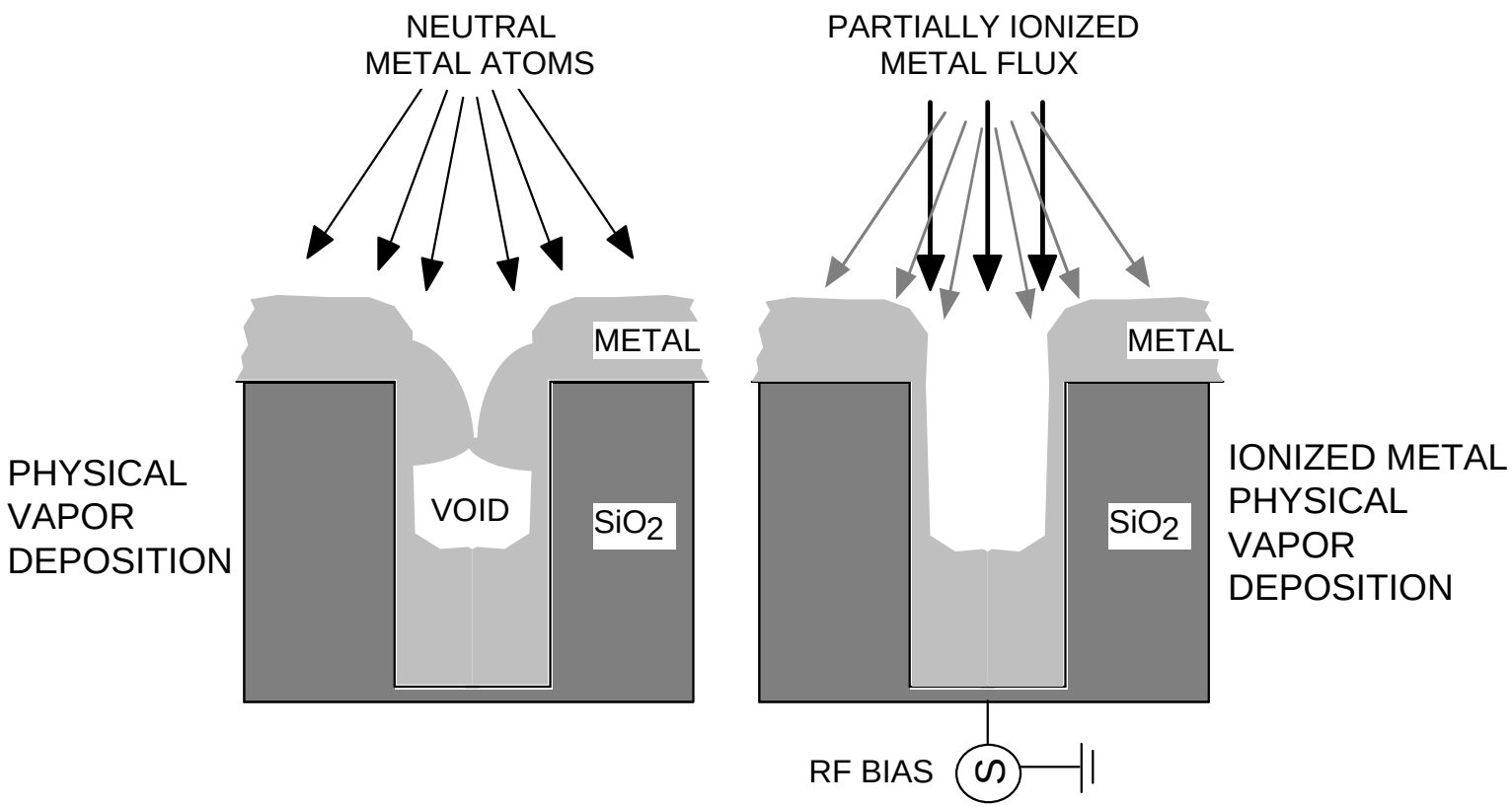
Typical Conditions:

- **10's mTorr Ar buffer**
- **100s V bias on target**
- **100s W - kW ICP**
- **10s V substrate bias**

University of Illinois
Optical and Discharge Physics

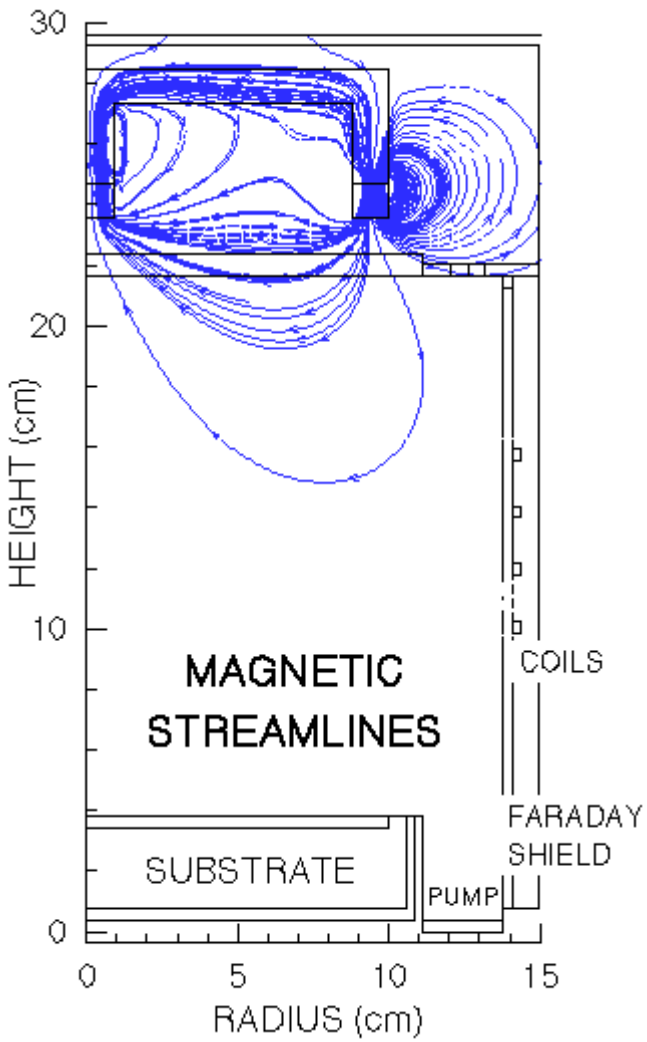
IONIZED METAL PHYSICAL VAPOR DEPOSITION

- **In Physical Vapor Deposition (PVD), the majority of the metal flux to the substrate is neutral, having a broad angular distribution. This leads to nonconformal deposition and creation of voids.**



- **In IMPVD, the addition of anisotropic metal ions to the flux produces conformal deposition by anisotropic filling and sputtering of overhangs.**

PVD/IMPVD OF Cu: REACTOR LAYOUT



- **PVD/IMPVD reactor with Cu Target**
  - **3.5- 20 mTorr Ar (constant pressure), 150 sccm**
  - **Annular magnetic field (200 G below target**
  - **Target: -200 V dc (2.4 kW)**
  - **Substate: 40 V, 10 MHz, 350 W**
  - **Coils: 2 MHz, 1250 W with Faraday shield**

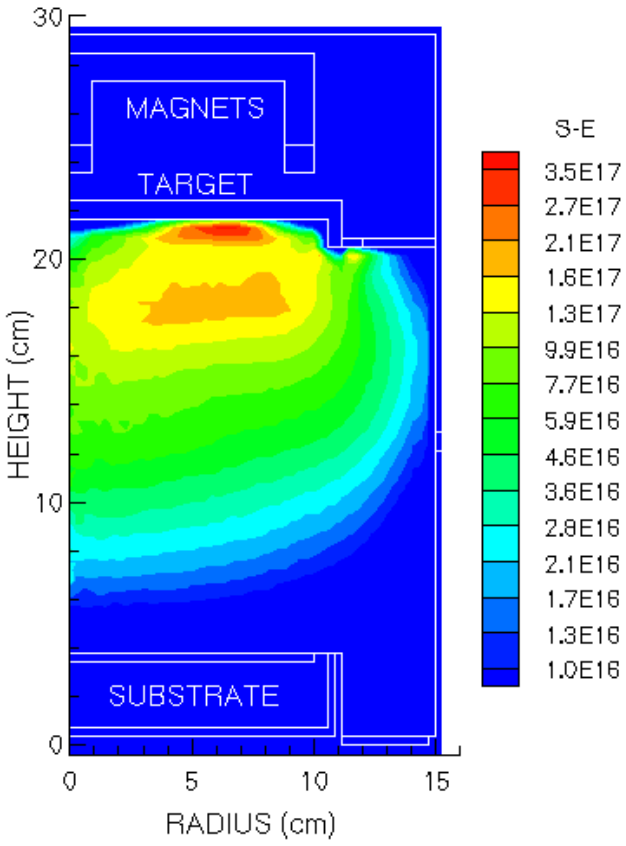
- **Physics included:**
  - **Gas heating by sputtered target atoms**
  - **Ion energy dependent sputter yield**
  - **Neutral and ion momentum and energy**
  - **Bulk electron energy equation**
  - **Monte Carlo secondary electrons**
  - **Cross field Lorentz forces**

MAGNETRON SPUTTER TOOL: Ar/Cu

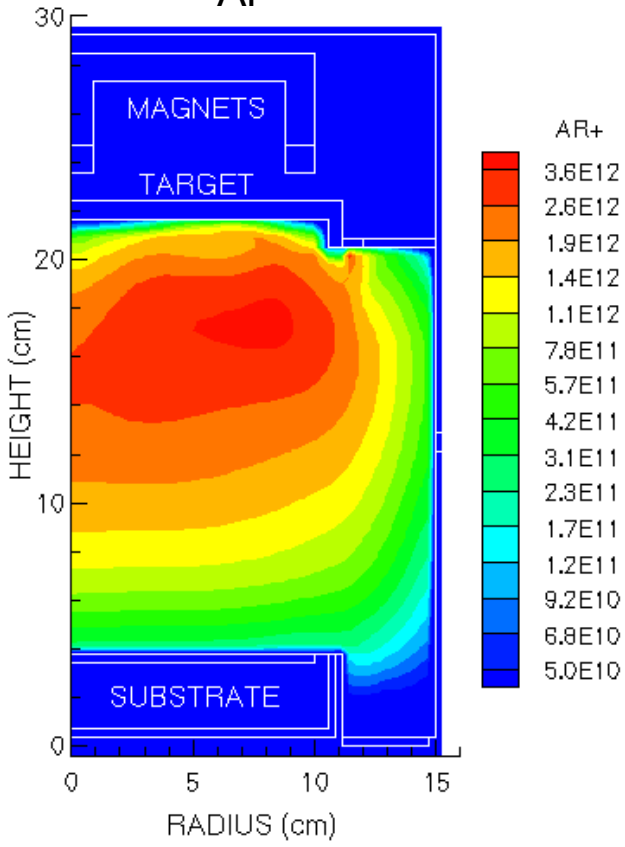
- Secondary electron emission from the target, and electron heating in the sheath, produces a torroidal electron source.

- Peak ion densities are mid-10^{12} cm^{-3}.

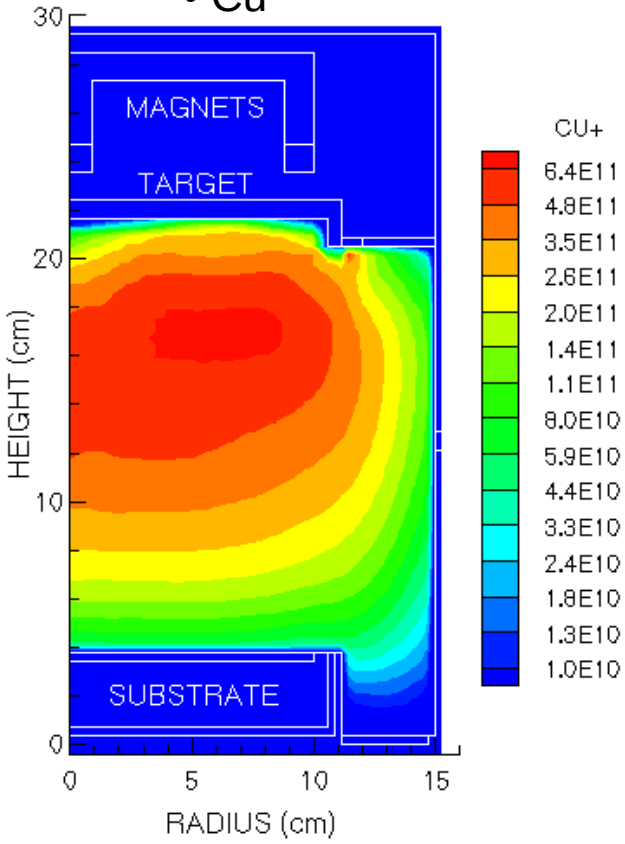
- e-Source



- Ar^+



- Cu^+



- Ar, 3.5 mTorr
- -200 V Target, 200 G

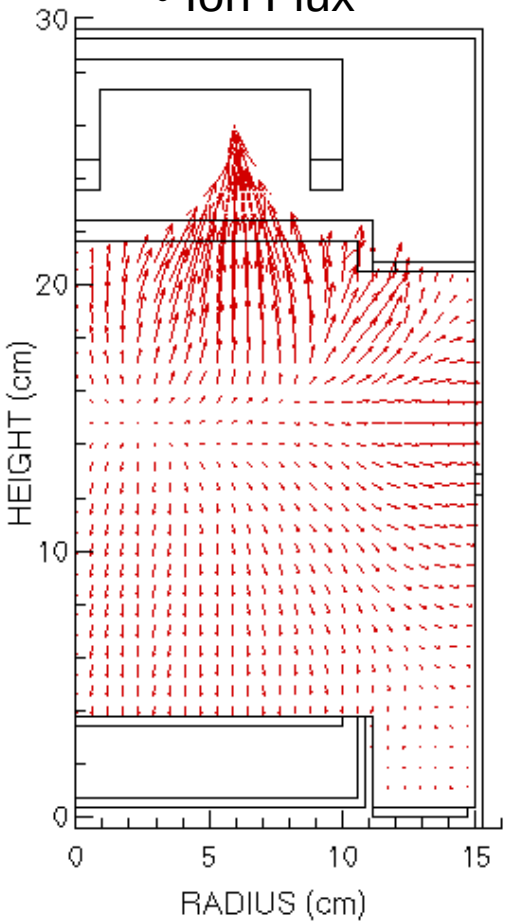
UNIVERSITY OF ILLINOIS
OPTICAL AND DISCHARGE PHYSICS

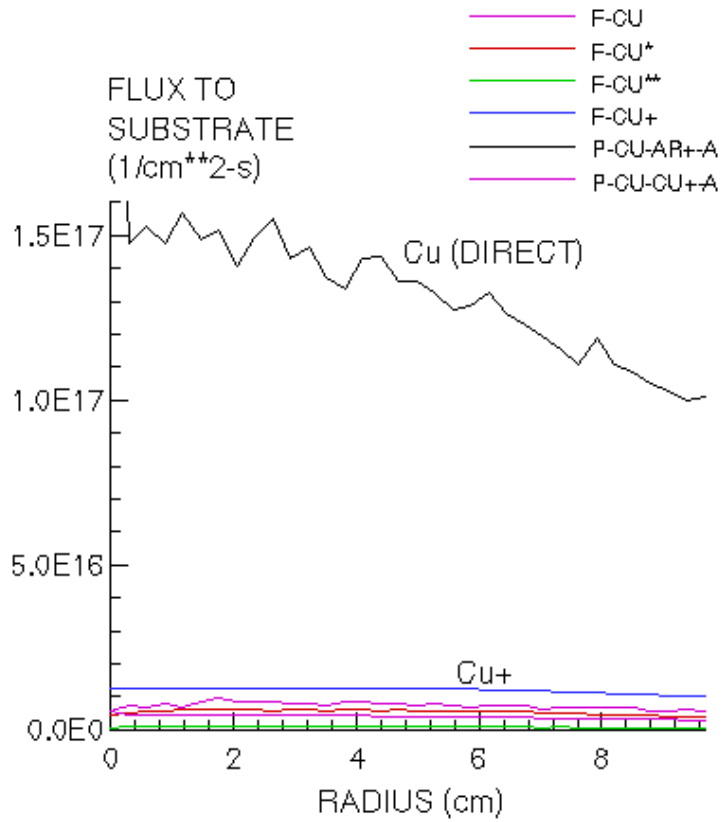
FLUXES IN THE Ar/Cu PVD TOOL

- Ion sputtering of the target produces a neutral Cu flux into the plasma.

- The low gas pressure and long mean free math of Cu atoms results in the flux to the substrate being “direct” neutrals.

- Ion Flux



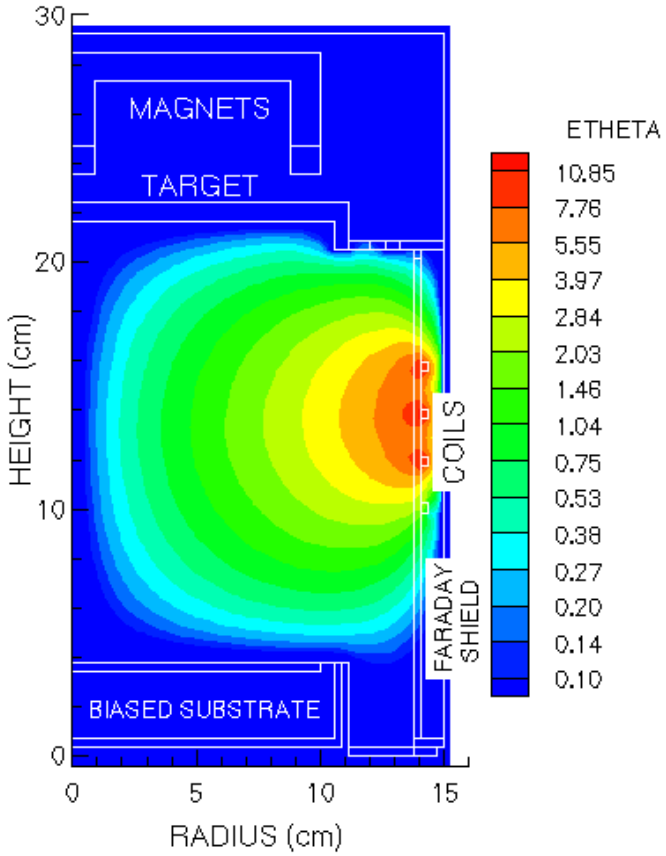


- Ar, 3.5 mTorr
- -200 V Target, 200 G

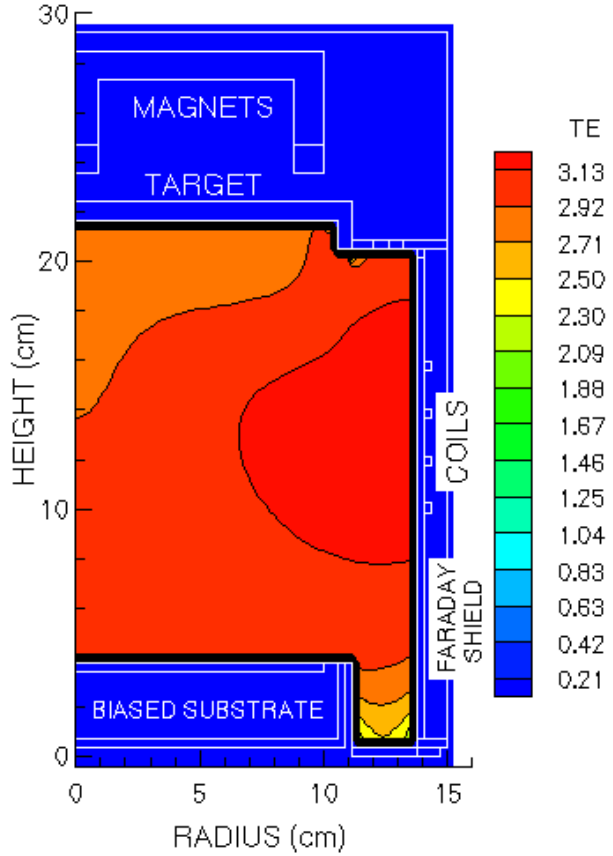
IMPVD TOOL: FIELDS AND TEMPERATURES

- The added inductively coupled electric field from the rf coils heats electrons in the bulk plasma producing a peak in temperature away from the target.

- Electric field



- Electron Temperature



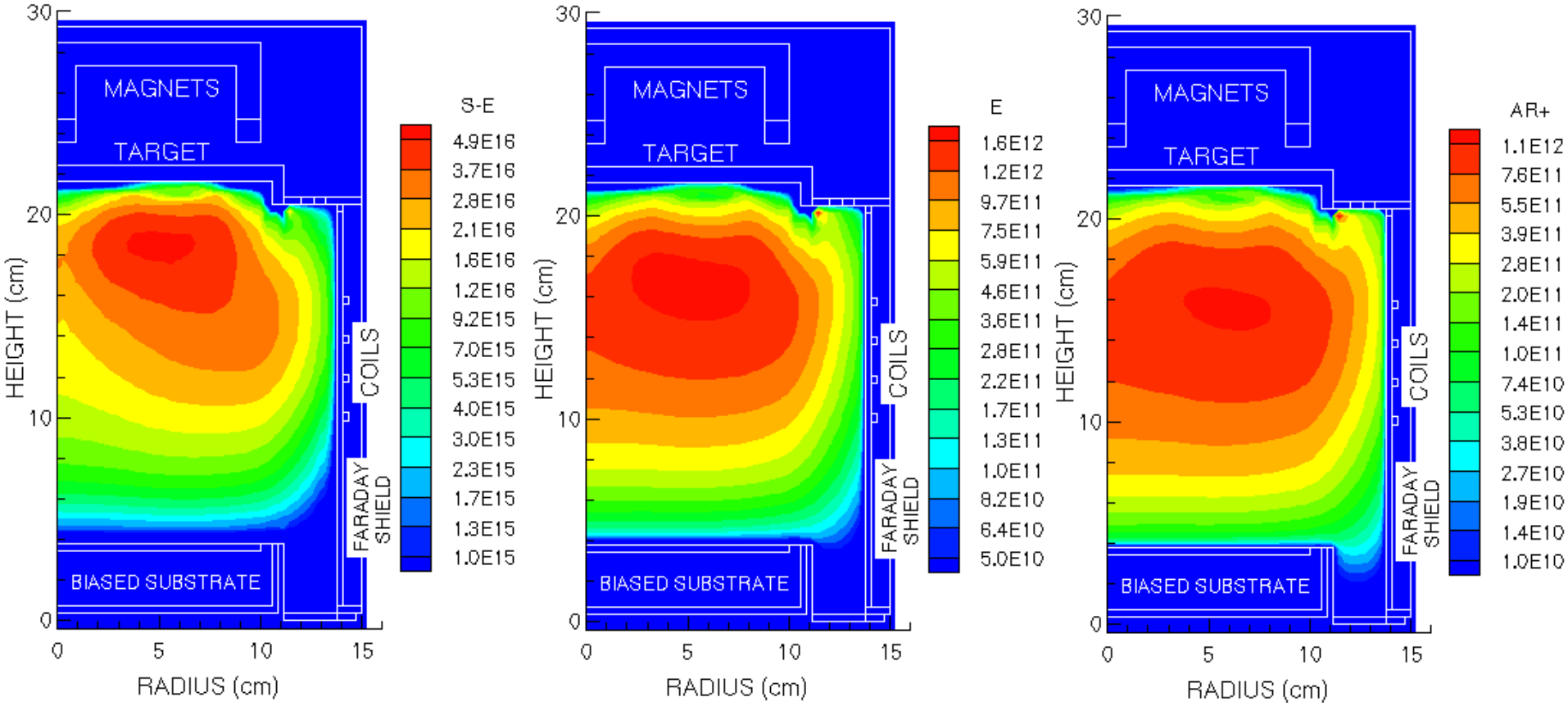
- Ar, 20 mTorr
- -200 V Target, 200 G
- 1.25 kW ICP, 2 MHz

UNIVERSITY OF ILLINOIS
OPTICAL AND DISCHARGE PHYSICS

IMPVD TOOL: ELECTRON SOURCE AND DENSITY

- The combination of the magnetron fields and heating from the rf coils produces a more extended electron source and electron density. The ion density is 75% argon.

- Electron Source
- Electron Density
- Ar^+



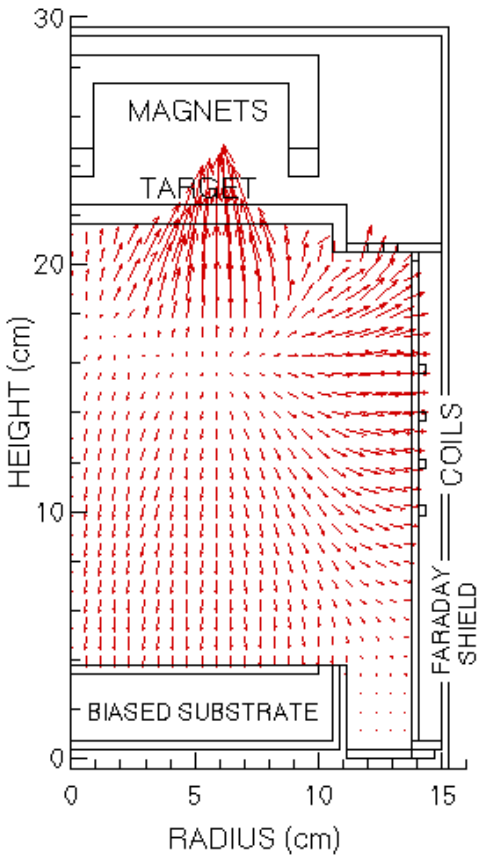
- Ar, 20 mTorr
- -200 V Target, 200 G
- 1.25 kW ICP, 2 MHz

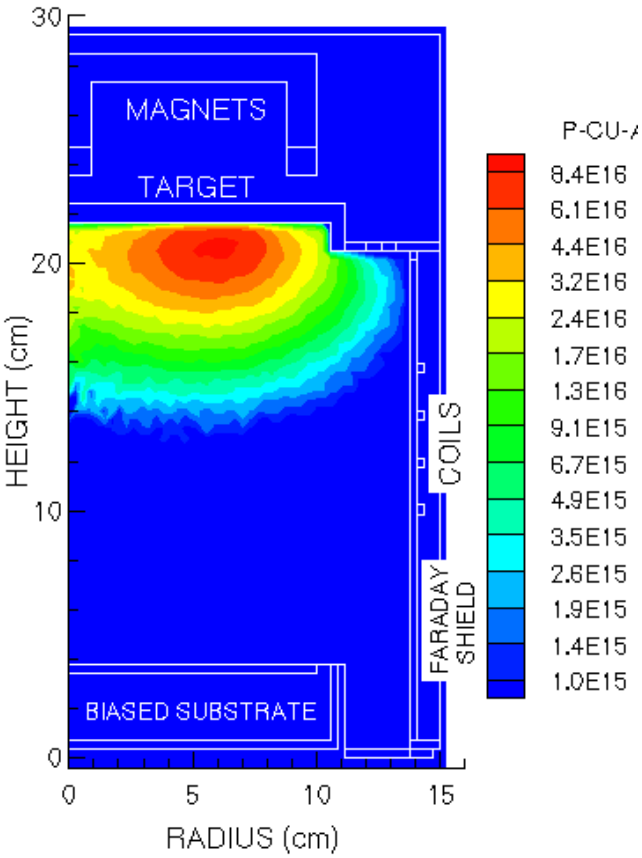
UNIVERSITY OF ILLINOIS
OPTICAL AND DISCHARGE PHYSICS

IMPVD TOOL: ION FLUX AND SPUTTER SOURCE

- The magnetron focus the ion flux to the target, producing a sputter source of Cu atoms.
- Due to the high gas pressure, the Cu atoms are thermalized in the vicinity of the target.

- Ion Flux





- Cu Source

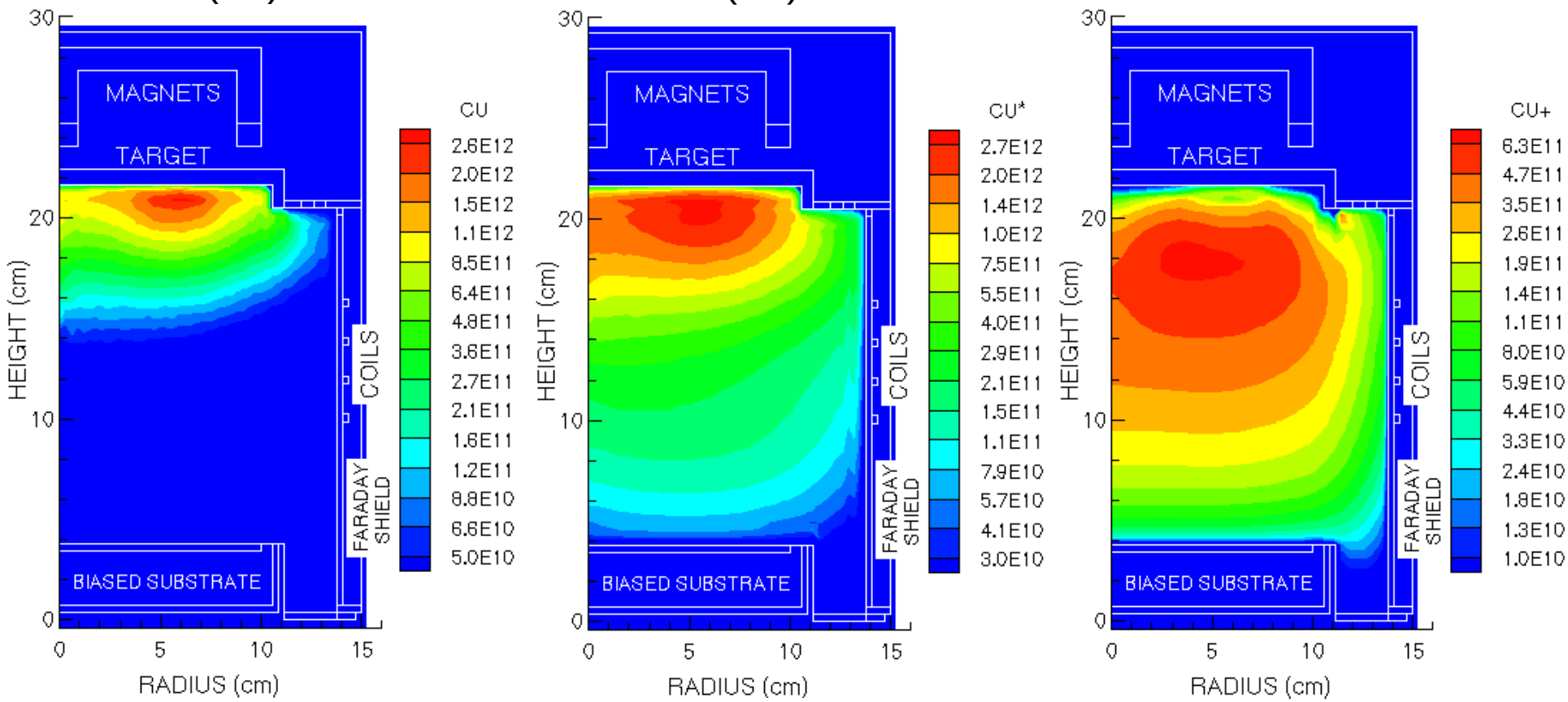
- Ar, 20 mTorr
- -200 V Target, 200 G
- 1.25 kW ICP, 2 MHz

UNIVERSITY OF ILLINOIS
OPTICAL AND DISCHARGE PHYSICS

IMPVD TOOL: Cu DENSITIES

- Due to the longer residence time of Cu in the chamber and the higher electron temperature produced by the rf heating, the Cu inventory is largely converted to ions and metastables [Cu(^{2}D)].

- Cu(^{2}S)
- Cu(^{2}D)
- Cu$^+$



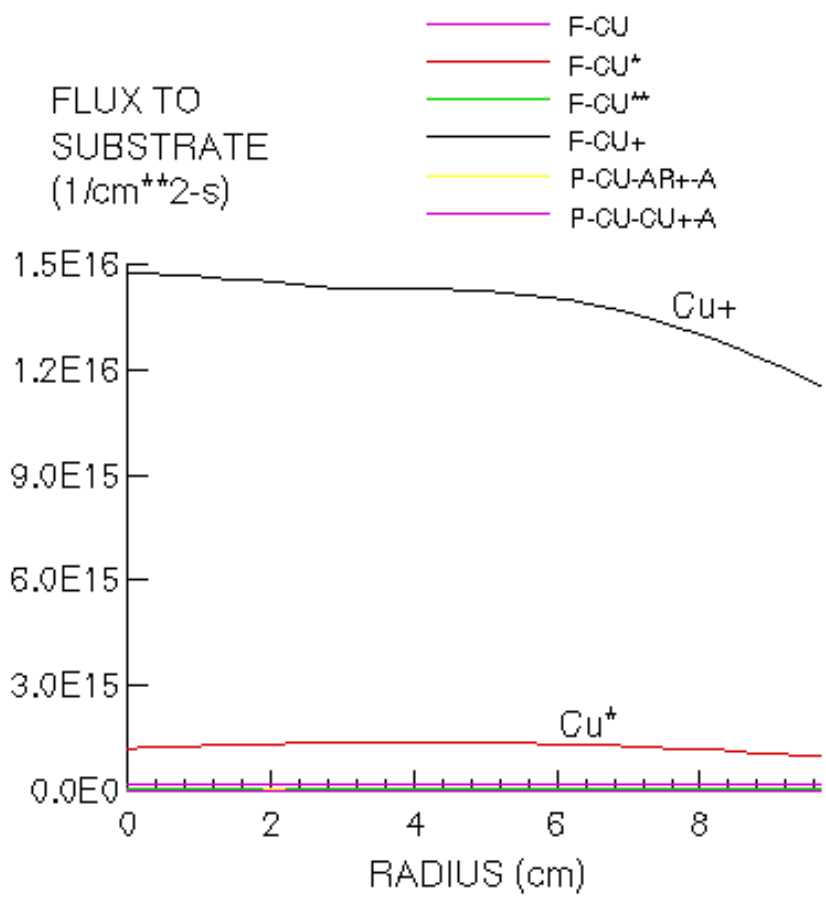
- Ar, 20 mTorr
- -200 V Target, 200 G
- 1.25 kW ICP, 2 MHz

UNIVERSITY OF ILLINOIS
OPTICAL AND DISCHARGE PHYSICS

IMPVD TOOL: Cu FLUXES TO SUBSTRATE

- The flux of Cu to the substrate is 85-90% ionized.
- The neutral flux is largely metastable Cu(^{2}D).

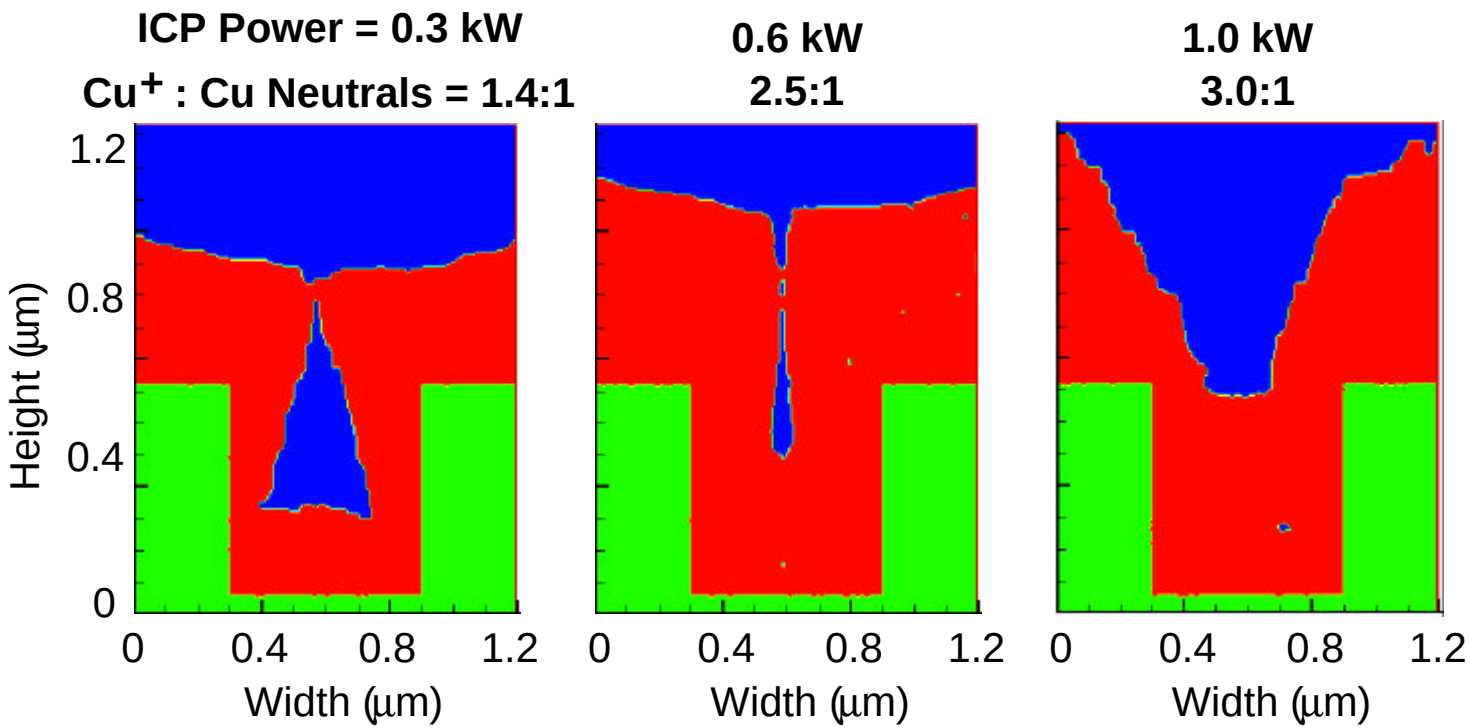
- Ar, 20 mTorr
- -200 V Target, 200 G
- 1.25 kW ICP, 2 MHz



TRANSITION FROM PVD TO IMPVD

- **With increasing ICP power deposition, a larger proportion of the Cu metal flux striking the substrate is ionized.**

- **The end result is conformal trench filling and elimination of the void.**

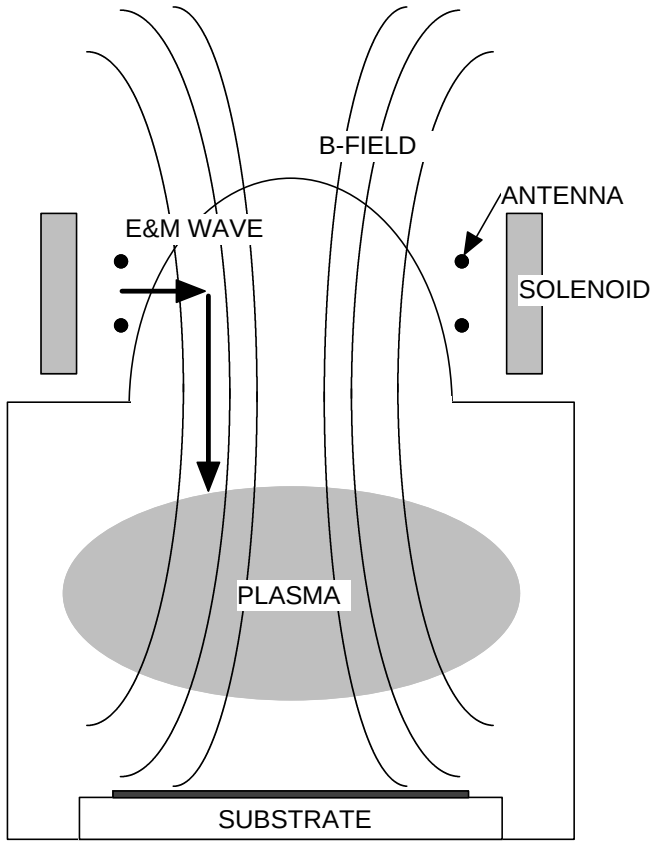


- **Ar 30 mTorr, 300 W Magnetron, -30 V bias**

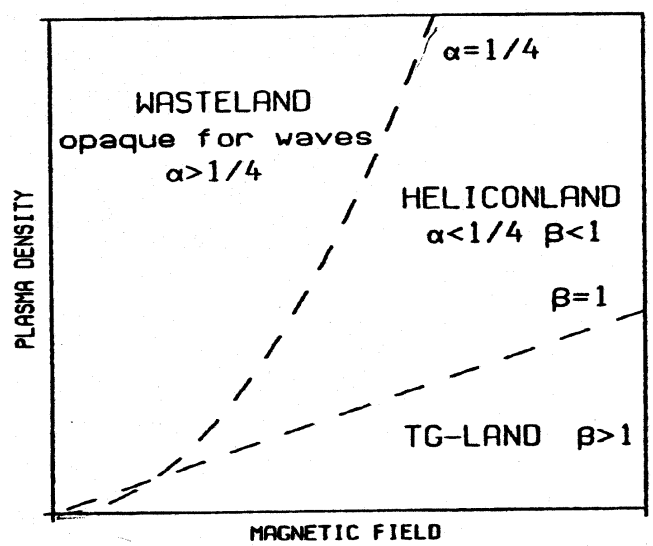
University of Illinois
Optical and Discharge Physics

WAVE PROPAGATION IN MAGNETICALLY ENHANCED ICPs

- **It is often desirable to produce plasmas in the "volume" of large reactors. This is difficult to accomplish using ICPs due to their finite skin depth.**
- **With a solenoidal magnetic field, electromagnetic waves can be made to propagate into the volume of the plasma.**



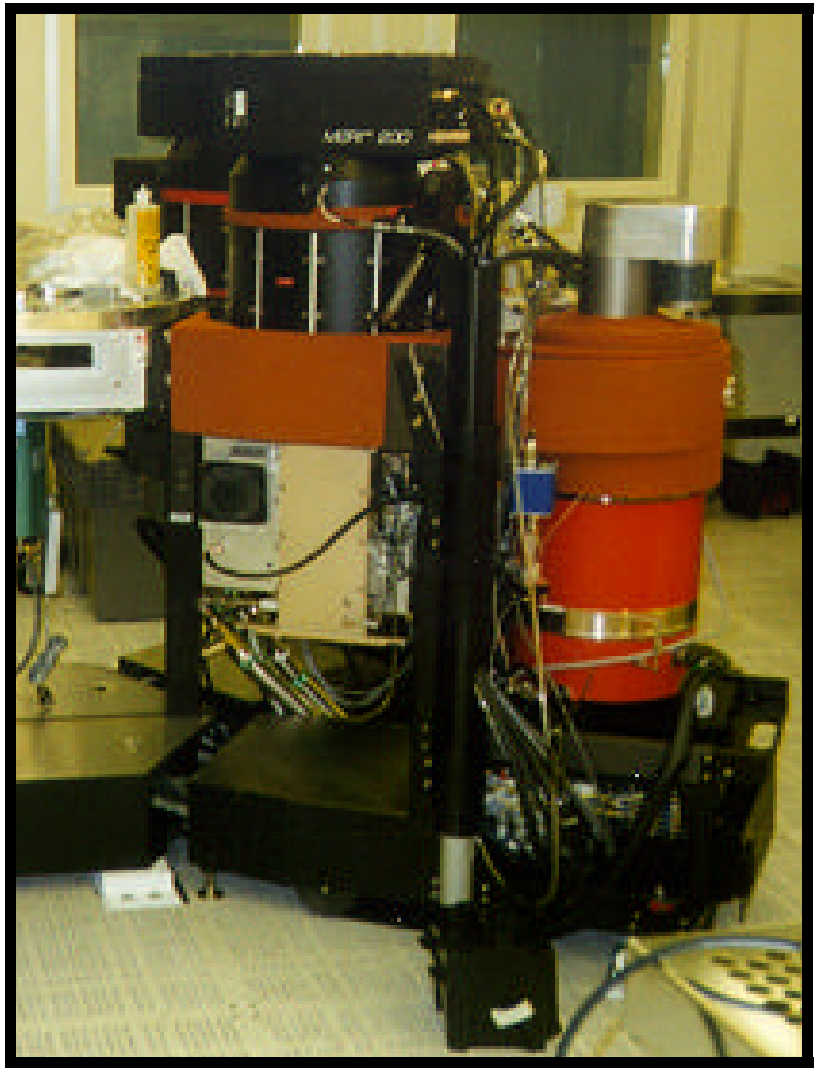
- **In magnetically enhanced ICP excitation occurs through electromagnetic and electrostatic modes.**
- **Helicon**
- **Trivelpiece-Gould**

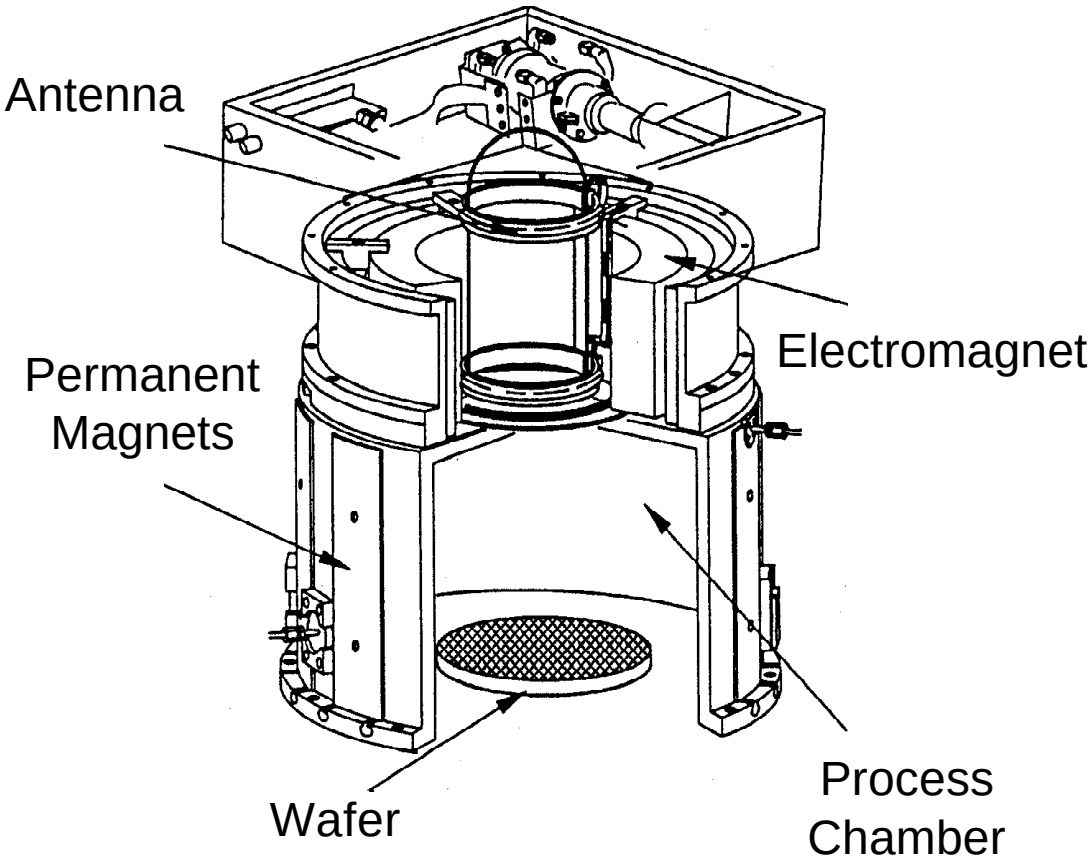


University of Illinois
Optical and Discharge Physics

TRIKON MORI™ 200 PLASMA TOOL

- **The HPEM was applied to analysis of a commercial MEICP etching tool.**



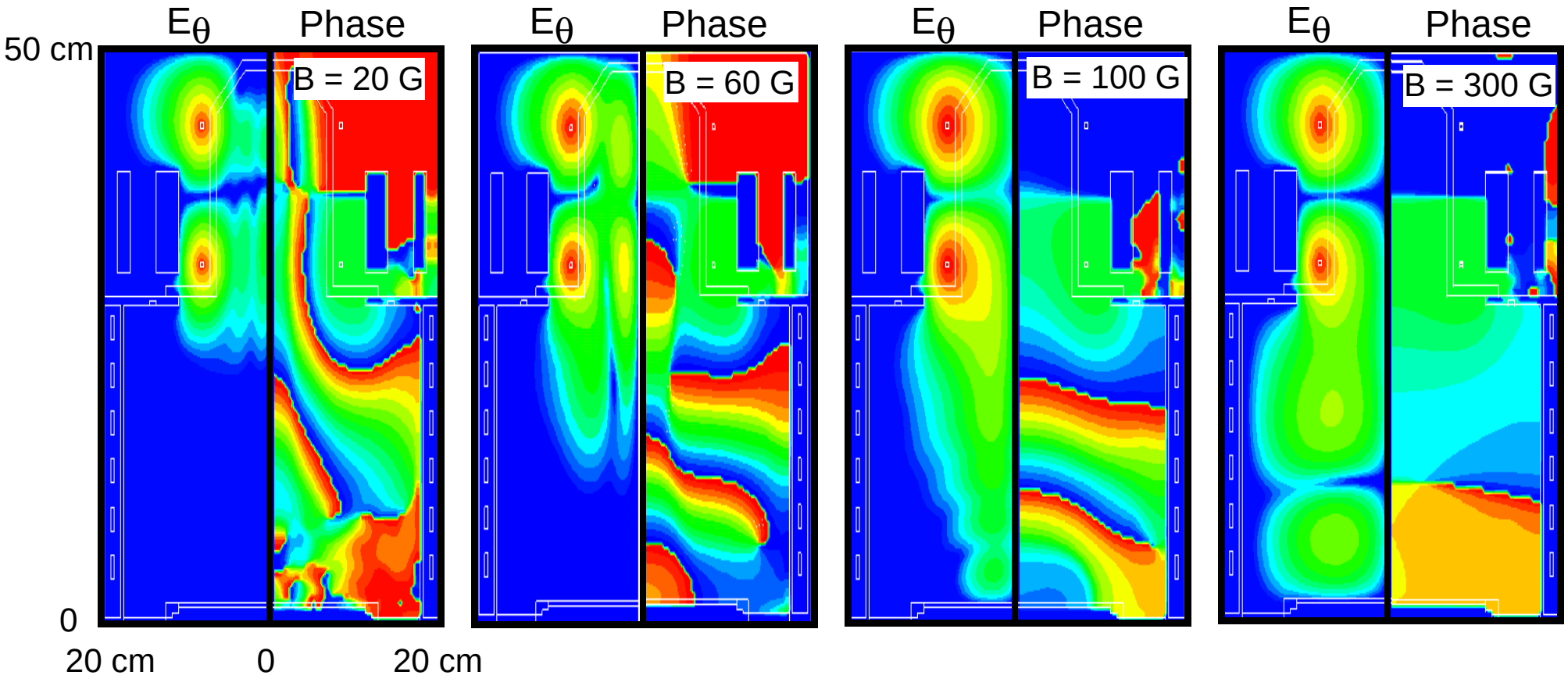


UNIVERSITY OF ILLINOIS
OPTICAL AND DISCHARGE PHYSICS

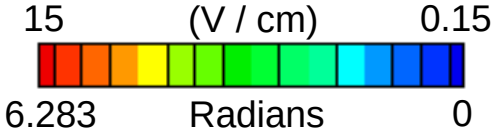
ANALYSIS OF TRIKON PLASMA TOOL : E_θ

- **At low B-fields, the electromagnetic propagation is mainly inwardly radial producing standing wave patterns.**

- **As the B-field increases, propagation shifts to the axial direction with increasing wavelength.**



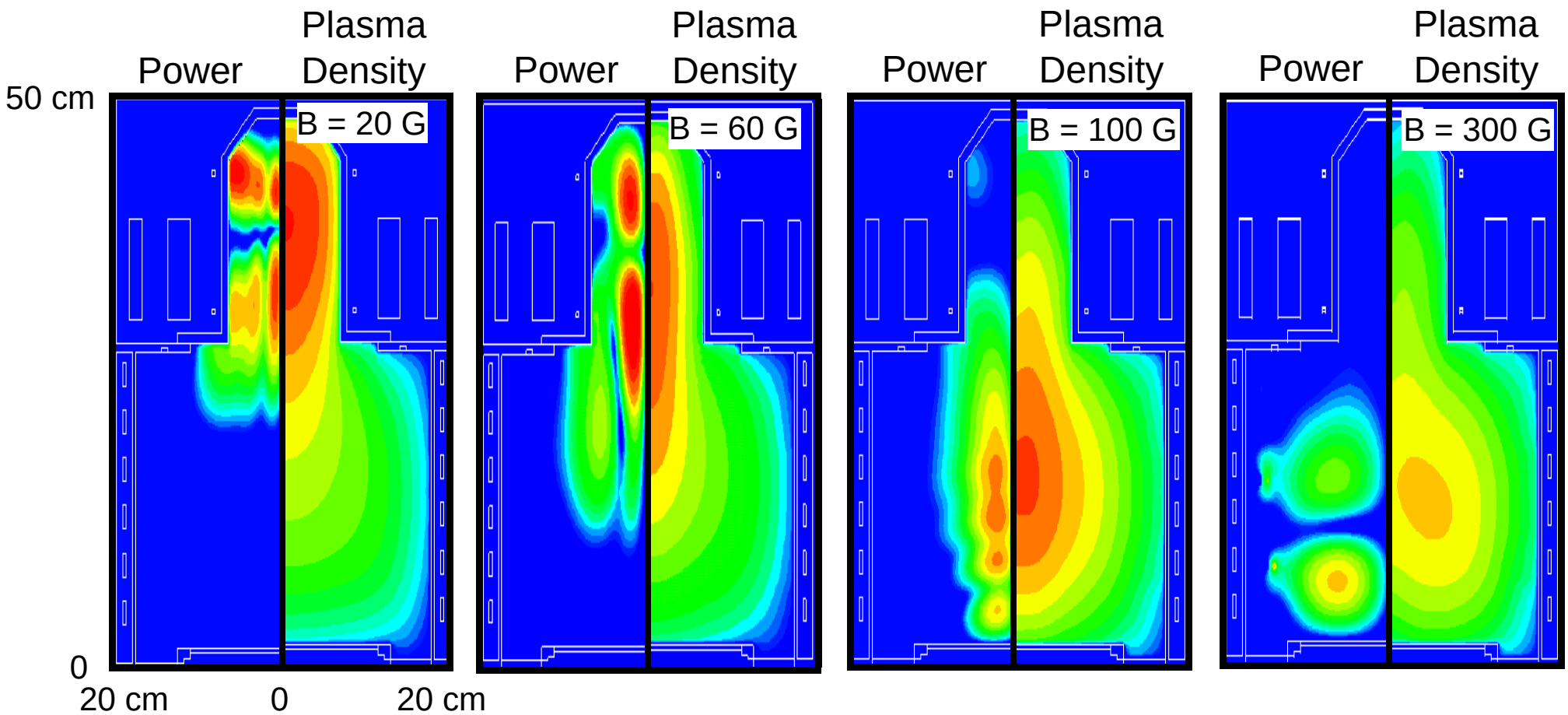
- **Ar, 10 mTorr, 1kW, 50 sccm**



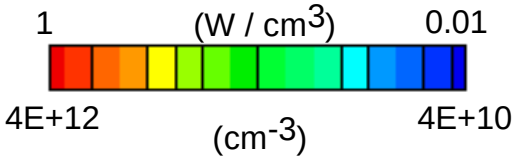
UNIVERSITY OF ILLINOIS
OPTICAL AND DISCHARGE PHYSICS

ANALYSIS OF TRIKON PLASMA TOOL : POWER AND ELECTRON DENSITY

- **As the magnetic fields increase, axial propagation dominates depositing power in the downstream region.**



- **Ar, 10 mTorr, 1kW, 50 sccm**



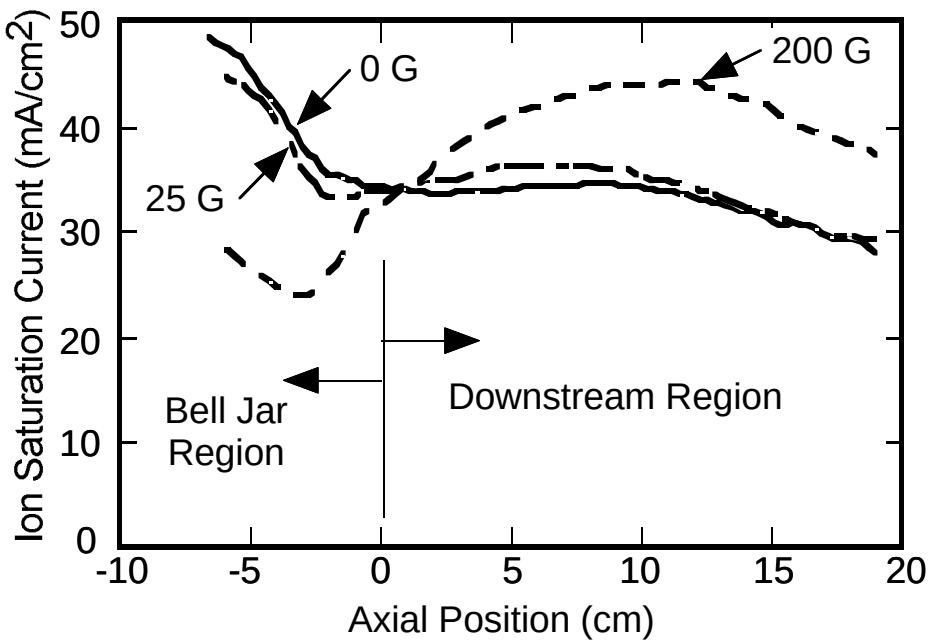
UNIVERSITY OF ILLINOIS
OPTICAL AND DISCHARGE PHYSICS

ANALYSIS OF TRIKON PLASMA TOOL: VALIDATION

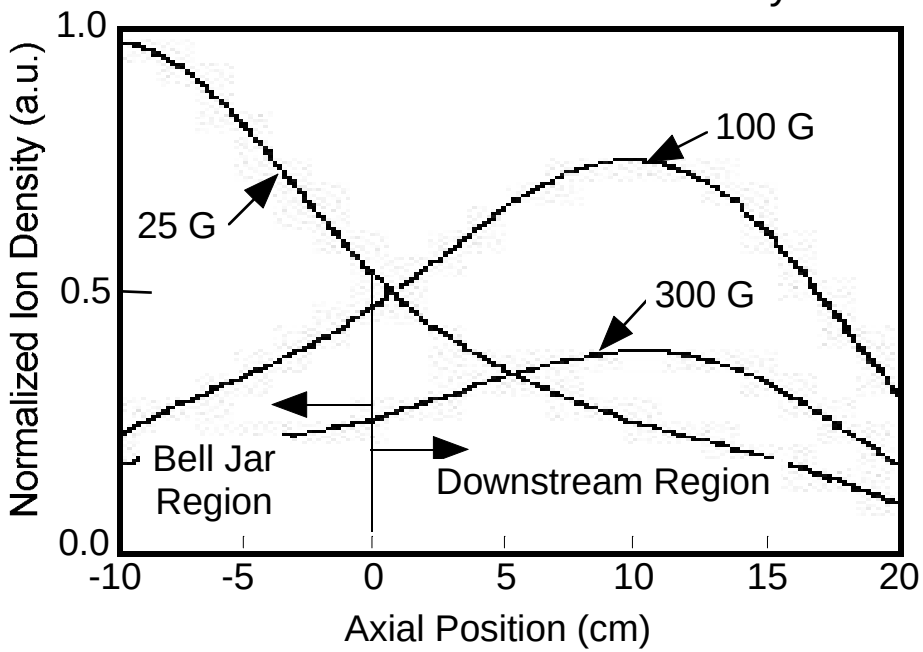
- **As the static magnetic field increases, the ion saturation current peaks further downstream.**

- **For constant power deposition, the peak downstream plasma density decreases due to the larger volume of the lower chamber.**

Experimental Axial Ion Saturation Profile



Theoretical Axial Ion Density



- **Ar, 2.3 mTorr, 1kW (Trikon Technologies, Inc.)**

- **Ar, 10 mTorr, 1kW, 50 sccm**

UNIVERSITY OF ILLINOIS
OPTICAL AND DISCHARGE PHYSICS

WAVELENGTH IN CYLINDRICAL GEOMETRY

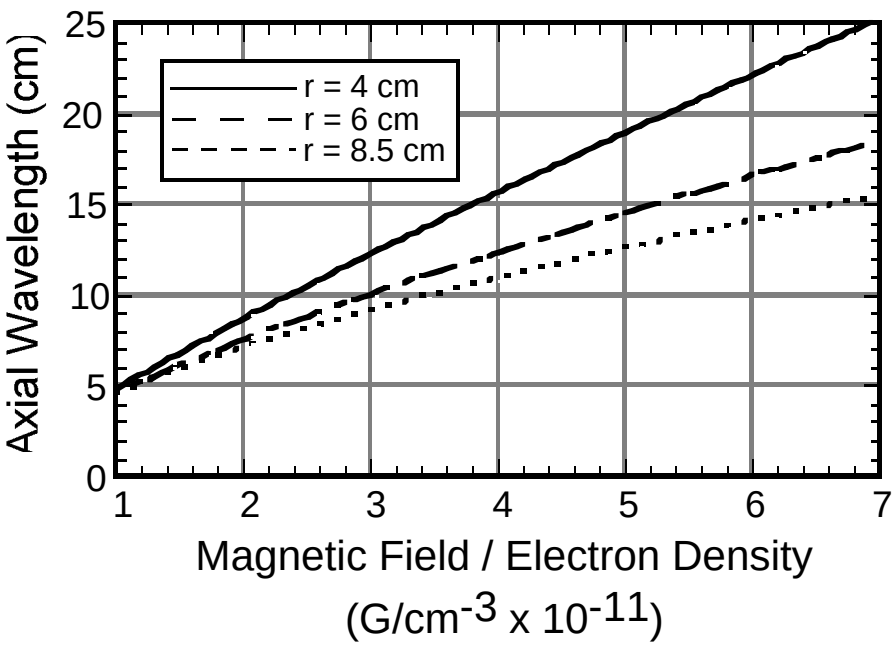
- **Using the dispersion relation for a helicon wave, the wavelength for an *m* = 0 mode can be obtained. From the simulation, the wavelength resembles an *m* = 0 in a cylindrical geometry.**

$$\lambda_z = \frac{3.83\, B_o}{R\, e\, \mu_o\, n_e\, f} \qquad \text{for } k_\perp >> k_z$$

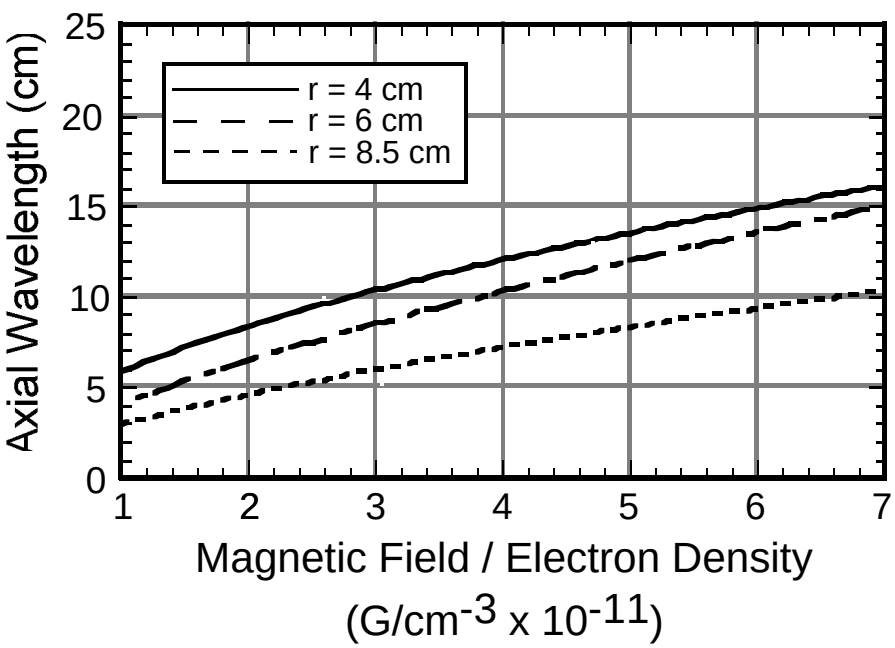
$$\lambda_z = \text{Sqrt}\left(\frac{2\, \pi\, B_o}{e\, \mu_o\, n_e\, f} \right) \qquad \text{for } k_z >> k_\perp$$

$$\lambda_{z\ (cm)} = \frac{7.6 \times 10^6}{R_{cm}} \left(\frac{B_o\ (\text{Gauss})}{n_{e\ (cm^{-3})}} \right)^{0.6}$$

Theoretical Wavelength



Computed Wavelength



UNIVERSITY OF ILLINOIS
OPTICAL AND DISCHARGE PHYSICS

AZIMUTHAL AND AXIAL ELECTRIC FIELDS

Azimuthal and axial components of the electric field will be shown for: Ar, 1 kW, 10 mTorr, B = 20-300 G

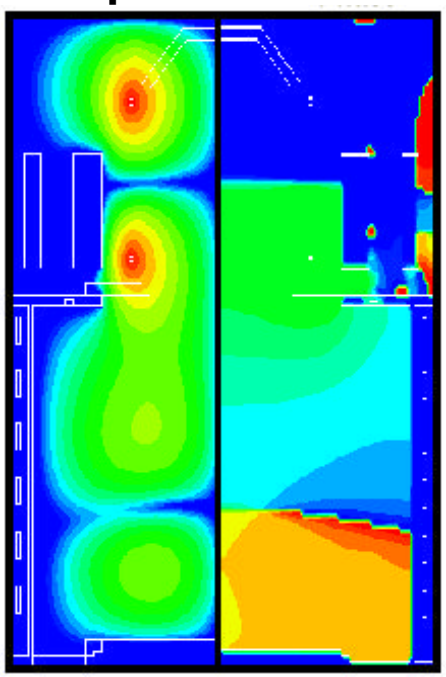
University of Illinois
Optical and Discharge Physics

DOWNSTREAM AXIAL COMPONENTS

- **With increaing B-field, the downstream electric field is increasingly dominated by axial and radial components.**
- **The end result is a large acceleration gradient in a direction of high mobility for conditions where the mean-free-path of electrons is large.**

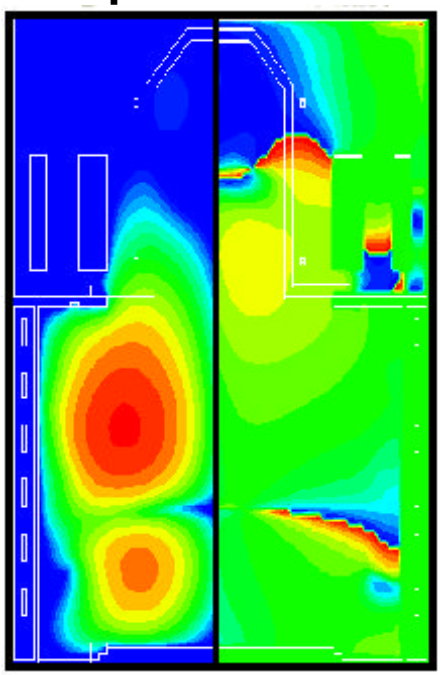
- **300 G, 1 kW, 10 mTorr**

Amplitude/Phase



E(θ) [0.15 - 15 V/cm]

Amplitude/Phase



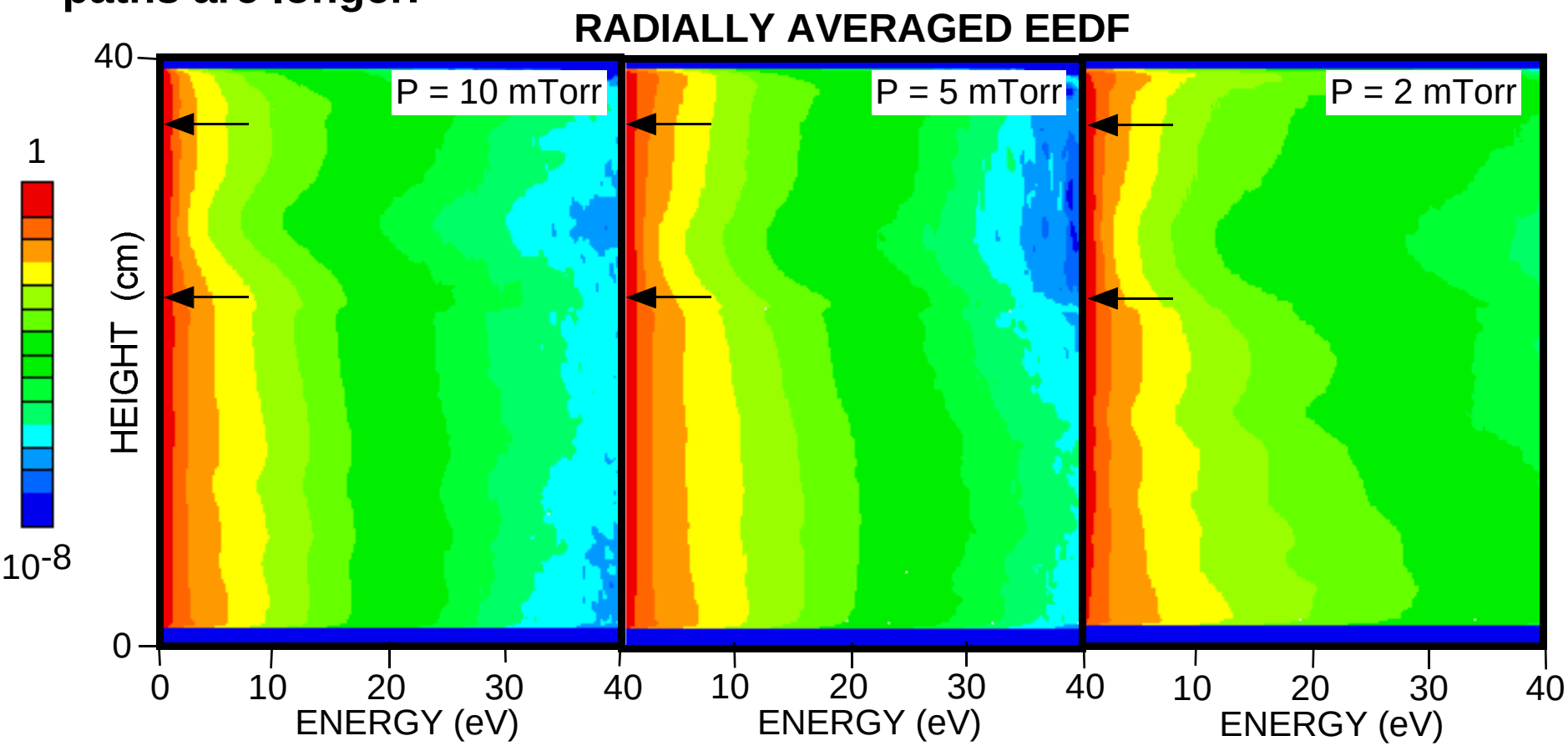
E(z) [0.05 - 5 V/cm]

University of Illinois
Optical and Discharge Physics

COLLISIONLESS HEATING

- **The long mean free path of electrons of 10s eV (while lower energy electrons are collisional) and the presence of axial electric fields downstream results in collisionless heating and some Landau damping.**

- **The effect is more pronounced at lower pressures where mean-free-paths are longer.**



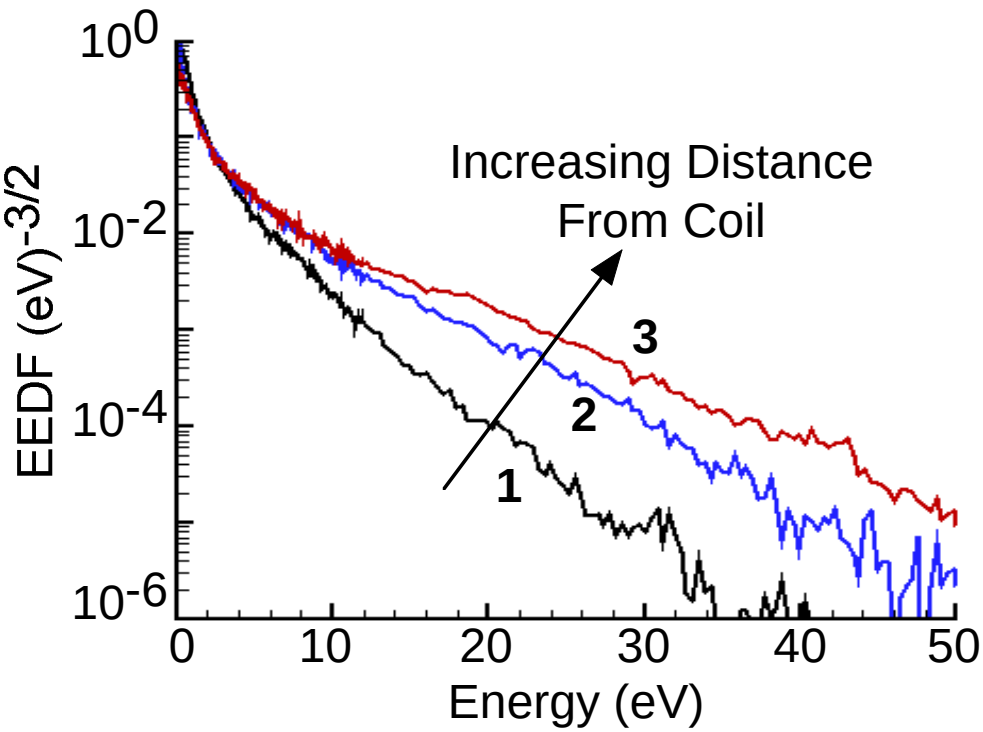
- Ar, 1 kW, 50 sccm, 300 G

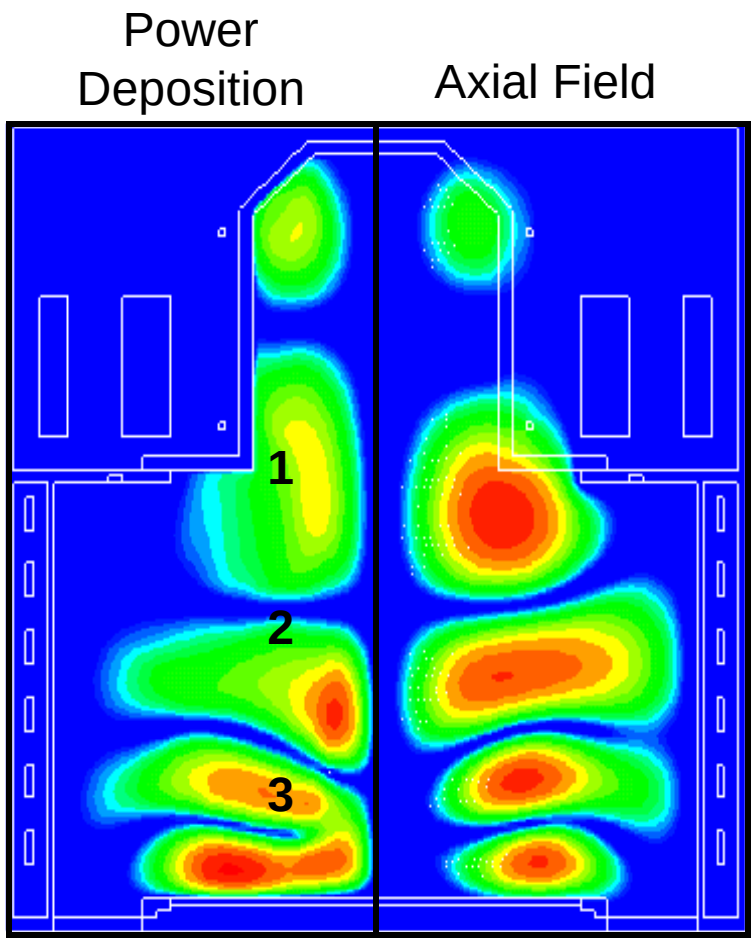
UNIVERSITY OF ILLINOIS
OPTICAL AND DISCHARGE PHYSICS

COLLISIONLESS HEATING

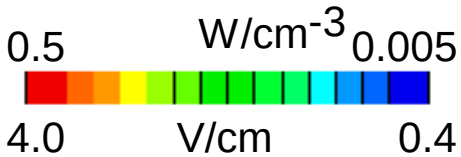
- **The tail end of the EED continues to "lift" with increasing distance downstream from the coils indicating some amount of electron trapping.**

- **The axial component of the electromagnetic field is responsible for most of the power deposition.**





- Ar, 1 kW, 300 G, 2mTorr



CONCLUDING REMARKS

- **Plasma equipment modeling has developed to the point that quantitative design of tools can be performed and the design cycle can be shortened.**
- **Process design based on modeling is in a more qualitative state, though progress is being made.**
- **Significant improvements are required in our databases of fundamental parameters (e.g., cross sections) so that more complex plasma chemistries can be addressed.**

University of Illinois
Optical and Discharge Physics