MODELING OF MICRODISCHARGE DEVICES: PLASMA AND GAS DYNAMICS*

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

October 2004

* Work supported by the National Science Foundation and Air Force Research Labs.
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.

\[
\lambda_D \approx 750 \left( \frac{T_e V}{n_e (cm^{-3})} \right)^{1/2} cm \approx 10 \mu m,
\]

\[
L_{\text{cathode fall}} = \left( \frac{2V_c \varepsilon_0}{qn_1} \right)^{1/2} \approx 10 - 20 \mu m
\]
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: Nonpdpstm 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:

\[
- \nabla \cdot \varepsilon \nabla \Phi = \rho_V + \rho_S
\]

- Photoionization, electric field and secondary emission:

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

\[
S_{si} = -\nabla \cdot j, \quad j_{E} = AT^2 \exp\left(\frac{-\left(\Phi_W - (q^3E/\varepsilon_0)^{1/2}\right)}{kT_S}\right), \quad j_S = \sum_j \gamma_{ij} \phi_j
\]
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.

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

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

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

- 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

\[ S_{Si} = \sum_j \left( \nabla \cdot \vec{\phi}_j \right) \gamma_{ij} \]
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 \( \Delta t \).

\[
N_i(t + \Delta t) = N_i(t) + \Delta N_i
\]

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

- 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.

\[
\begin{bmatrix}
\text{Charged Particles and Potential} \\
\Rightarrow \text{Electron Temperature} \\
\Rightarrow \text{Neutral Densities} \\
\Rightarrow \text{Surface Chemistry}
\end{bmatrix}_{\Delta t_1} 
\rightarrow 
\begin{bmatrix}
\text{Electron Monte Carlo}
\end{bmatrix}_{\Delta t_2} 
\rightarrow 
\begin{bmatrix}
\text{Electron Transport Coefficients}
\end{bmatrix}_{\Delta t_3} 
\rightarrow 
\begin{bmatrix}
\text{Electromagnetics}
\end{bmatrix}_{\Delta t_4} 
\rightarrow 
\begin{bmatrix}
\text{Navier Stokes} \\
\text{Neutral Densities}
\end{bmatrix}_{\Delta t_5}
\]

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

- MDs with 10s - 100s $\mu$m 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
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)
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
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
Peak electron densities of $>10^{14}$ cm$^{-3}$ are produced in the steady state.

These high cw densities enable large rates of excitation of high lying electronic states.
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.

\[ \text{Visible Emission Ar}(4p) \ (10^{13} \text{ cm}^{-3}) \]

\[ \text{Excimer Emission } \text{Ar}_2^* \ (10^{11} \text{ cm}^{-3}) \]

- **Ar**(4p) Density (Visible Emission)
- **Ar\(_2^*\)** Density (UV Emission)
• 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**
• 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**

University of Illinois
Optical and Discharge Physics
- Beam Ionization

- Electron Density

**MD PROPERTIES vs PRESSURE**

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

- The result is more confinement at higher pressure and higher peak electron density.

- Ar, 2 mA

- 125 Torr $1.3 \times 10^{14}$

- 250 Torr $2.1 \times 10^{14}$

- 500 Torr $3.5 \times 10^{14}$
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

University of Illinois
Optical and Discharge Physics
Experimental trends are reproduced for contraction of optical emission with increasing pressure.

- Ref: Maria Cristina Penache, Thesis, 2002
• Large metastable densities produce efficient excimer emission at higher pressures.

• Ref: Maria Cristina Penache, Thesis, 2002

• Ar, 2 mA

University of Illinois
Optical and Discharge Physics
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
The end result is a more tightly confined plasma at the lower pressure.

- 0.15 mA
- 4.0 mA
MD PROPERTIES vs CURRENT: $T_{\text{gas}}, [e]$

- 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.
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.

Ref: Maria Cristina Penache, Thesis, 2002

University of Illinois
Optical and Discharge Physics
SENSITIVITY TO $\gamma$ (SECONDARY EMISSION): $[e]$

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

- $\gamma = 0.05$

- $\gamma = 0.20$

University of Illinois
Optical and Discharge Physics
• Voltage and peak electron density increases with decreasing $\gamma$ to counter smaller flux of beam electrons which ionize efficiently.

• Power increases when holding current constant.

- Ar, 250 Torr, 2 mA
Visible emission increases as $\gamma$ decreases, in part reflecting increase in power.

Distribution of emission also shifts to being more dominated by beam electrons.

• Ar, 250 Torr, 2 mA
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
• 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
• 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
MD AS A RADICAL SOURCE: He/O$_2$

- Large current densities and intrinsically high gas flow makes MDs ideal for reactant generators. Demonstrate with electronegative He/O$_2$ mixture.

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

- He/O$_2$=90/10, 125 Torr, 2 mA
MD SUSTAINED IN He/O\textsubscript{2}: ELECTRON SOURCES

- \( S(\text{beam}) \)
- \( T_e \)
- \( S(\text{bulk}) \)

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

- He/O\textsubscript{2}=90/10, 125 Torr, 2 mA
MD SUSTAINED IN He/O\textsubscript{2}: ELECTRON, ION DENSITIES

- [e]
- [N\textsuperscript{+}]
- [N\textsuperscript{-}]

- Negative ions are dominated by O\textsubscript{2}\textsuperscript{-} at pressures of 100s Torr.

- He/O\textsubscript{2}=90/10, 125 Torr, 2 mA
The range of O atoms is limited by recombination and ozone formation. $O_2(^1\Delta)$ and $O_3$ are final products, having longer ranges.

Cataphoresis induced flow preferentially ejects reactants downward.

- $He/O_2=90/10$, 125 Torr, 2 mA

University of Illinois
Optical and Discharge Physics
In spite of Frank-Condon heating, gas temperatures are lower (for a given current) than in argon due to higher thermal conductivity of He.

- He/O\textsubscript{2}=90/10, 125 Torr, 2 mA
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.


University of Illinois
Optical and Discharge Physics
MODEL GEOMETRY: Si PYRAMID MICRODISCHARGE

- Investigations of a cylindrically symmetric Si pyramid microdischarge were performed.
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 MΩ
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 $\mu$m, 200 V, 1 M$\Omega$
TRANSITION TO NEGATIVE-GLOW BEHAVIOR

- Although geometry precludes true hollow cathode behavior, negative glow behavior sets in at lower pressures.

- Characterize negative glow by $\frac{S[\text{Ne}^2^+] }{(S[\text{Ne}^+] + S[\text{Ne}^2^+] )}$

- Ne, 50 $\mu$m diameter, 200 V, 1 M$\Omega$

University of Illinois
Optical and Discharge Physics
SCALING WITH PRESSURE: PLASMA PROPERTIES

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

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

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

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

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

- Ne, 50 µm diameter, 200V, 1 MΩ

University of Illinois
Optical and Discharge Physics
SCALING CONSIDERATIONS: CATHODE FALL THICKNESS

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

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

- $210 \, \text{V}, \, 1 \, \text{M}\Omega$
  $[e]= 4.9 \times 10^{13} \, \text{cm}^{-3}$

- $200 \, \text{V}, \, 1.75 \, \text{M}\Omega$
  $[e]= 5.3 \times 10^{12} \, \text{cm}^{-3}$

- Ne, 50 $\mu$m diameter, 600 Torr

University of Illinois
Optical and Discharge Physics
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
SCALING WITH SIZE: \( pd, j = \text{CONSTANT} \)

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

\[ [e] \text{ (Max } = 2.96 \times 10^{13} \text{ cm}^{-3}) \]

- 400 Torr
- 600 Torr
- 1000 Torr

- Ne, -200 V

University of Illinois
Optical and Discharge Physics
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.