Simulation of an Atmospheric Pressure Direct Current Microplasma Discharge in He/N₂

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1. Atmospheric pressure glow discharge
2. Plasma simulation using COMSOL Multiphysics
3. He/N$_2$ dc microplasma model
4. Results
   - Current-voltage (I-V) characteristics
   - Discharge structure such as cathode dark space (CDS) region
   - Effect of cathode temperature
5. Conclusions
Recently, interest has grown toward atmospheric pressure plasmas to reduce the cost by moving away from vacuum equipment.

Microplasmas are characterized by their small size (characteristic dimensions, of tens to hundreds of microns) and high gas pressure (100 Torr–1 atm), yielding nonequilibrium plasmas.
Atmospheric pressure glow discharge (2)

Application fields

- Etching for semiconductor devices
- Formation of Diamonds
- Formation of carbon nanotube
- Flue gas treatment
- Ozone formation
- Sterilization, etc.
- Control of physicochemical properties on substrate
- Biocompatibility granted to medical materials

In this work,

The atmospheric pressure direct current (dc) microdischarge, one of the easy methods of generating an atmospheric pressure nonequilibrium plasma, is studied.
The common types of plasma:

- Inductively coupled plasma (ICP)
- DC discharge
- Microwave plasma
- Electrical breakdown
- Capacitively coupled plasma (CCP)
- Combined ICP/CCP reactor
Plasma module physics interfaces

- The drift diffusion interface
- The heavy species transport interface
- The Boltzmann equation, Two-term approximation interface
- The inductively coupled plasma interface (ICP)
- The microwave plasma interface
- The capacitively coupled plasma interface (CCP)
- The DC discharge interface
Plasma module format in COMSOL Multiphysics

Plasma interfaces

Plasma model library
### Plasma chemistry

#### Neutrals (2)

- He, N₂

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#### Ions (3)

- He⁺, He₂⁺, N₂⁺

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#### Excited species (3)

- He(2¹S), He(2³S), He⁺

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<table>
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<th>No.</th>
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<tr>
<td>2</td>
<td>e⁻ + He → e⁻ + He(2³S)</td>
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<td>3</td>
<td>e⁻ + He → 2e⁻ + He⁺</td>
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<td>4</td>
<td>e⁻ + He(2¹S) → 2e⁻ + He⁺</td>
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<td>6</td>
<td>2e⁻ + He⁺ → e⁻ + He</td>
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<td>7</td>
<td>2e⁻ + He⁺ → e⁻ + He⁺</td>
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<tr>
<td>8</td>
<td>e⁻ + He₂⁺ → He + He⁺</td>
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<tr>
<td>9</td>
<td>e⁻ + N₂ → 2e⁻ + N₂⁺</td>
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<td>10</td>
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<td>11</td>
<td>He⁺ + 2He → He₂⁺ + He</td>
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<td>12</td>
<td>He(2¹S) + He → 2He + hv</td>
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<td>He(2³S) + 2He → He₂ + He</td>
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<td>He(2³S) + He(2³S) → He⁺ + He + e⁻</td>
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<td>15</td>
<td>He⁺ + N₂ → N₂⁺ + He</td>
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<td>16</td>
<td>He₂⁺ + N₂ → N₂⁺ + 2He</td>
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<tr>
<td>17</td>
<td>He⁺ + N₂ + He → N₂⁺ + 2He</td>
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<tr>
<td>18</td>
<td>He₂⁺ + N₂ + He → N₂⁺ + 3He</td>
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<tr>
<td>19</td>
<td>He(2³S) + N₂ → N₂⁺ + He + e⁻</td>
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<td>20</td>
<td>He(2¹S) + N₂ → N₂⁺ + He + e⁻</td>
</tr>
<tr>
<td>21</td>
<td>He(2³S) + N₂ + He → N₂⁺ + 2He + e⁻</td>
</tr>
</tbody>
</table>
COMSOL Multiphysics solves a pair of drift diffusion equation for the electron density and electron energy density.

\[
\frac{\partial}{\partial t}(n_e) + \nabla \cdot \Gamma_e = R_e
\]

\[
\frac{\partial}{\partial t}(n_\varepsilon) + \nabla \cdot \Gamma_\varepsilon + E \cdot \Gamma_e = R_\varepsilon
\]

\[
\Gamma_e = -n_e(\mu_e E) - D_e \nabla n_e
\]

\[
\Gamma_\varepsilon = -n_\varepsilon(\mu_\varepsilon E) - D_\varepsilon \nabla n_\varepsilon
\]

Source term

\[
R_e = \sum_{j=1}^{M} x_j k_j N_n n_e
\]

Source term

\[
R_\varepsilon = \sum_{j=1}^{P} x_j k_j N_n n_e \Delta \varepsilon_j
\]

Rate coefficient

\[
k_j = \gamma \int_{0}^{\infty} \varepsilon \sigma_j(\varepsilon) f(\varepsilon) d\varepsilon
\]

\[
\gamma = (2q/m)^{1/2}
\]
Electron transport boundary conditions

- There are a variety of boundary conditions available for the electrons:
  - Wall which includes the effects of:
    - Secondary electron emission
    - Thermionic emission
    - Electron reflection
  - Flux which allows you to specify an arbitrary influx for the electron density and electron energy density.
  - Fixed electron density and mean electron energy
  - Insulation
Heavy species transport

- Transport of the heavy species (non-electron species) is determined from solving a modified form of the Maxwell-Stefan equations:

\[ \rho \frac{\partial}{\partial t} (w_k) + \rho (u \cdot \nabla) w_k = \nabla \cdot j_k + R_k \]

where

\[ j_k = \rho \omega_k v_k \]

\[ v_k = \sum_{j=1}^{Q} D_{kj} d_k - \frac{D_k^T}{\rho \omega_k} \nabla \ln T \]

\[ d_k = \frac{1}{cRT} \left[ \nabla p_k - \omega_k \nabla p - \rho_k g_k + \omega_k \sum_{j=1}^{Q} \rho_j g_j \right] \]

- The multiphysics interfaces contain an integrated reaction manager to keep track of the electron impact reactions, reactions, surface reactions and species.
Heat transfer inside the computational domain is modeled by the below equation:

\[ \rho c_p \frac{dT}{dt} + \nabla \cdot (-k \nabla T) = Q + q_s T - \rho c_p \mathbf{u} \cdot \nabla T + \tau : \mathbf{S} + \frac{T}{\rho} \left( \frac{\partial \rho}{\partial T} \right)_p \left( \frac{\partial p_a}{\partial T} + \mathbf{u} \cdot \nabla p_a \right) \]
Electrostatic field

- The plasma potential is computed from Poisson’s equation:

\[-\nabla \cdot \varepsilon_0 \varepsilon_r \nabla V = \rho\]

- The space charge is computed from the number densities of electrons and other charged species.

\[\rho = q \left( \sum_{k=1}^{N} Z_k n_k - n_e \right)\]

Discharge voltage

\[V_d = V - jAR_b\]

Electrode area

Discharge voltage

Ballast resistor

Current density

Supplied voltage
He/N$_2$ dc microplasma model (1)

Computational conditions

- Gas: pure He and He/N$_2$ mixtures
- N$_2$ fractions: 0.002–0.02%
- Pressure: 760 Torr
- Power source: DC
- Operating voltage: 232–450V
- Ballast resistor: 10 kΩ
- Electrode area: 0.006 cm$^2$
- Cathode temperature: 350, 450, 550 K
- Anode temperature: 350 K
He/N$_2$ dc microplasma model (2)

Coupled simulation of plasma and heat transfer

Plasma

Heat transfer

- Thermal conductivity
- Density
- Mass-averaged mixture specific heat
- Heat source
He/N\textsubscript{2} dc microplasma model (3)

PDE equation

\[ V_d = V - jAR_b \]

Plasma

Electric potential:
\[ V_0, V_d \]

Discharge voltage

\[ e_s \frac{\partial^2 V_d}{\partial t^2} + d_s \frac{\partial V_d}{\partial t} = f \]

Source Term
\[ f = V_d - V_0 + \text{abs}(dc.Jex + dc.Jix_wHe2_1p + dc.Jix_wHe1p + dc.Jix_wN2_1p)^A0*Rb \]
The boundary condition for electric field calculation is specified as $V_c = 0$ on the cathode and $V_a = V_d$ on the anode.
Results (2)

Discharge structure in a He/0.02%N\textsubscript{2} microdischarge at $V = 420$ V

Electrical potential and electron temperature

Number density

- Electron
- $\text{He}^+$
- $\text{He}_2^+$
- $\text{N}_2^+$
The effect of cathode temperature in He/0.02%N$_2$ microdischarges

The electrical conductivity $\sigma$ is strongly dependent on temperature, which can be approximated by

$$\sigma = \frac{1}{\rho_0 [1 + \alpha (T - T_0)]}$$
Discharge structure in He/0.02%N$_2$ microdischarges at different cathode temperatures

**Electrical potential**

- He/0.02%N$_2$ (350K)
- He/0.02%N$_2$ (450K)
- He/0.02%N$_2$ (550K)

**Electron density (m$^{-3}$)**

- He/0.02%N$_2$ (350K)
- He/0.02%N$_2$ (450K)
- He/0.02%N$_2$ (550K)
Results (5)

$I$-$V$ characteristics in He/0.02%N$_2$ microdischarges at different cathode temperatures
Conclusions

- The simulations of atmospheric pressure direct current microplasma discharges in He/N$_2$ were performed by coupling plasma simulation with heat transfer calculation.
- A simple circuit model was used to obtain the discharge voltage regarded as the boundary potential condition in the plasma simulation.
- The effect of a small amount of N$_2$ added to He as well as the effect of cathode temperature on the $I$-$V$ characteristics were studied.
- It could be concluded that by using COMSOL Multiphysics, the simulations would be very beneficial in finding the design parameters of atmospheric pressure plasma sources for surface modification.
Thank you for your attention