HYBRID GLOBAL MODEL SIMULATIONS OF He/N_2 AND He/H_2O ATMOSPHERIC PRESSURE CAPACITIVE DISCHARGES

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OUTLINE

- He/0.1%N_2 discharge with simplified chemistry
  - — Particle-in-cell (PIC) simulations (hours to days)
  - — Use PIC to develop fast hybrid global model (two electron temperatures + sheaths)
  - — Hybrid global model simulations (30 seconds)
  - — Electron multiplication in sheaths $\Rightarrow$ α-to-γ transition

- He/H_2O bounded discharge with complex chemistry
  - — Depletion of H_2O, reaction product diffusion
  - — Hybrid model simulations (two minutes)
  - — α-to-γ transition including depletion/diffusion effects

He/N_2 DISCHARGE

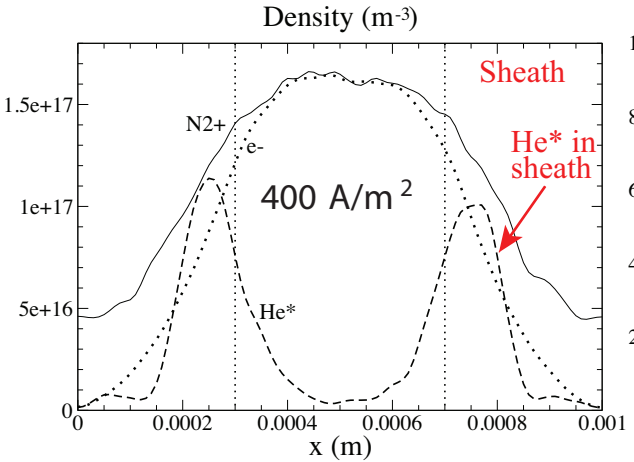
(Kawamura et al, PSST 23, 035014, 2014)

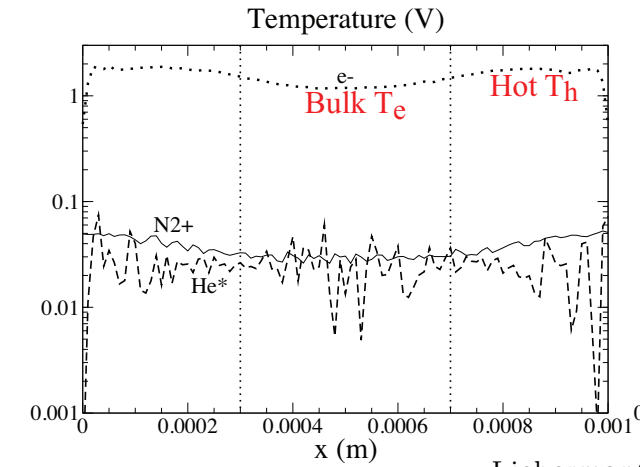
- Helium with 1000 ppm nitrogen at 760 Torr
- 1D plane-parallel geometry with 1 mm gap
- Current driven at 13.56–40.68 MHz, $J = 400$–6000 A/m^2
- Simplified reaction set with fixed He and N_2 densities:

  $e + He \rightarrow e + He$, Elastic Scattering
  $e + N_2 \rightarrow e + e + N_2^+$, Ionization
  $e + N_2^+ \rightarrow N + N$, Recombination (N is not followed in the PIC)
  $N_2^+ + He \rightarrow N_2^+ + He$, Ion Elastic Scattering
  $e + He \rightarrow e + He^*$, Metastable Excitation
  $He^* + 2He \rightarrow He_2^* + He$, Loss of He^* (He_2^* is not followed in the PIC)
  $He^* + N_2 \rightarrow e + N_2^+ + He$, Penning Ionization by He^*
  $He^* + He \rightarrow He^* + He$, He^* Elastic Scattering

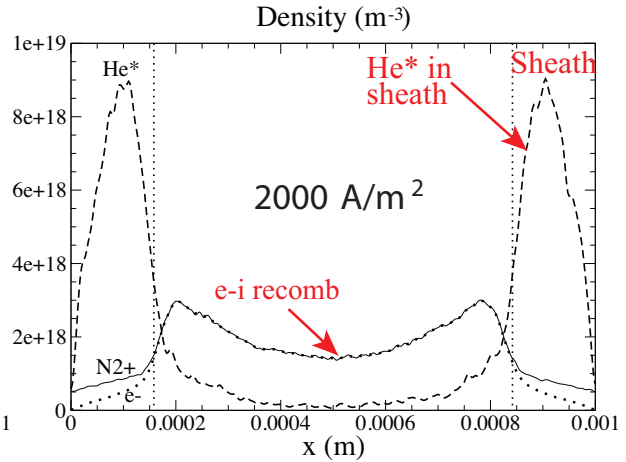
PIC RESULTS (27.12 MHz, 1 mm gap, 1000 ppm N_2)

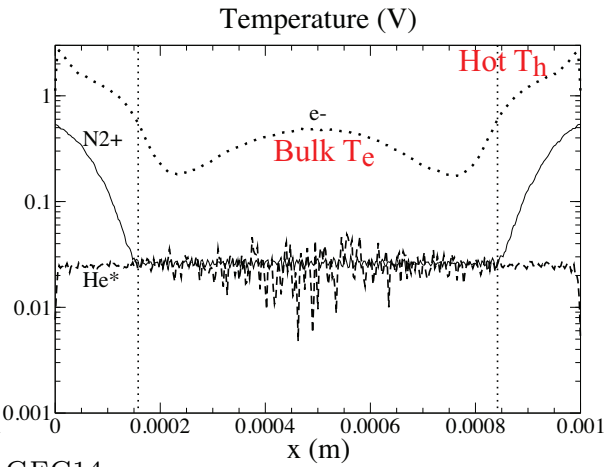
α-mode





γ-mode

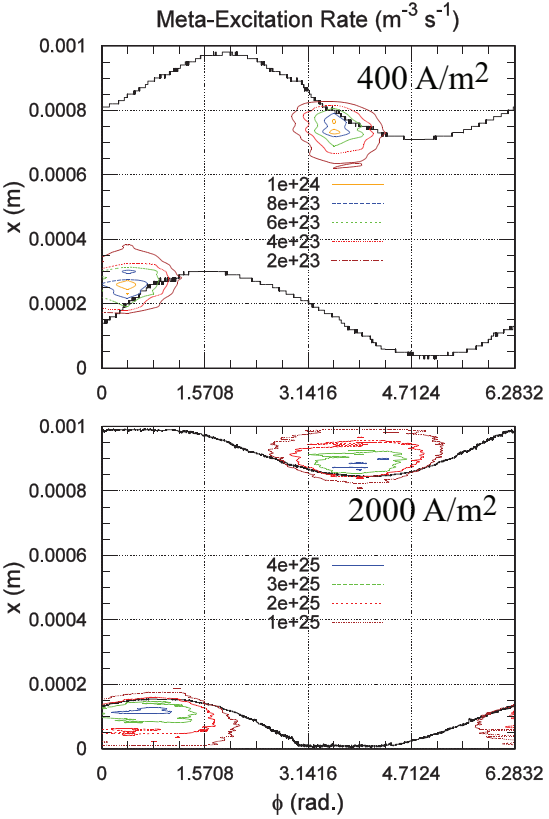


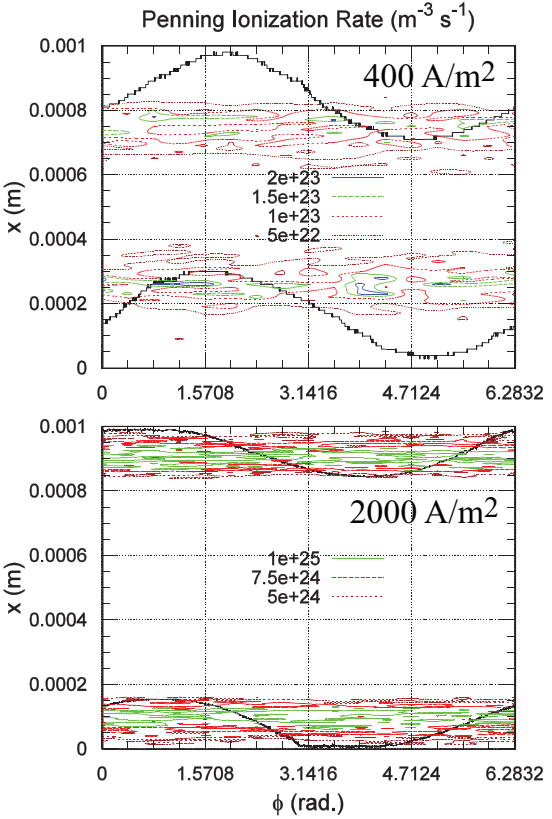


PIC RESULTS (cont'd)

α-mode

γ-mode





- Half of Penning ionization in high-field sheath region in γ-mode

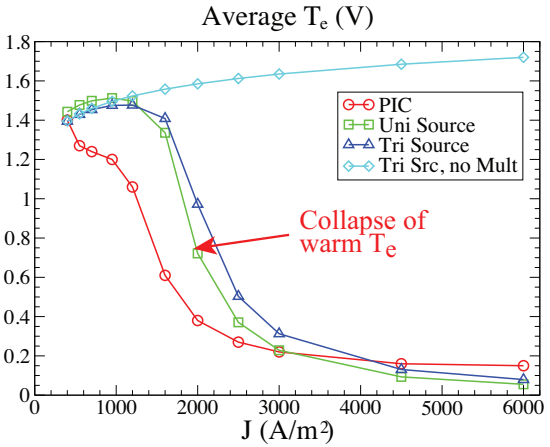
He/N_2 HYBRID MODEL ASSUMPTIONS

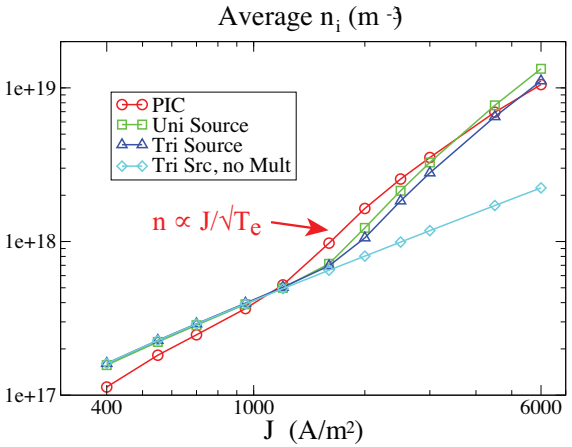
- Homogeneous discharge model for $E(z,t)$ and $s(t)$ (analytic)
- Electron power balance in bulk determines warm $T_e(t)$ (analytic) (ohmic power $J \cdot E \approx$ e-He elastic scattering power loss)
- E/n_{He} in sheaths determines hot $T_h(t)$ (analytic, BOLSIG+)
- Time-average over oscillating temperatures gives warm and hot electron rate coefficients (analytic, BOLSIG+)
- Uniform or triangular ion source profile within Child law sheath determines the mobility-driven ion wall losses (analytic)
- Secondary and Penning multiplication factors (numerical)
- Particle balance relations (numerical, using MATLAB `ode15s`)

$\Rightarrow$ Fast solution of discharge equilibrium

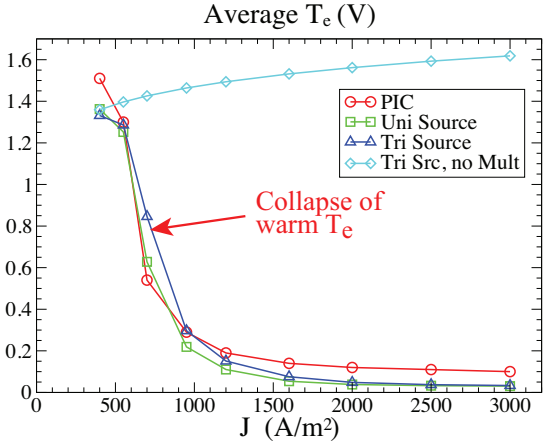
HYBRID MODEL – PIC COMPARISON

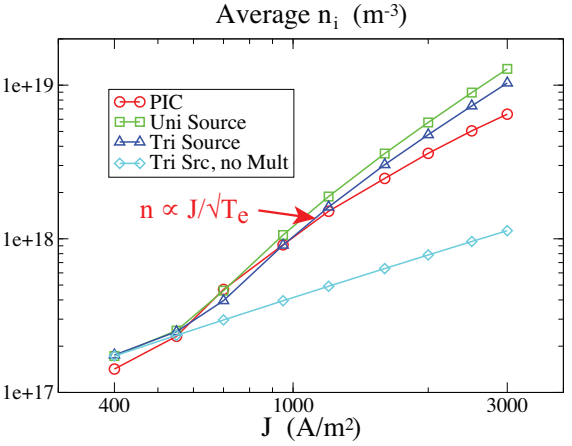
27.12 MHz





13.56 MHz



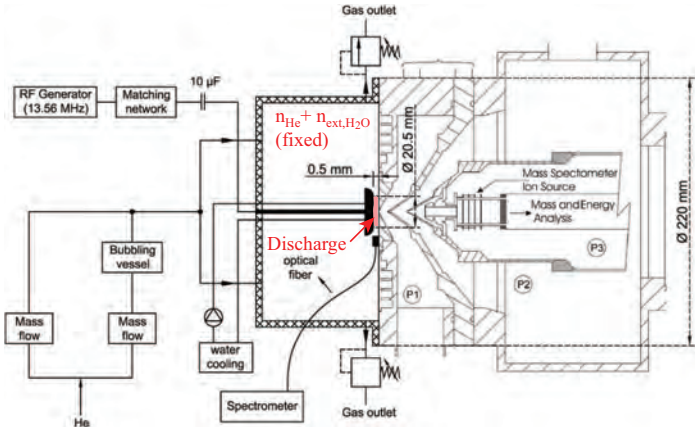


- Field at wall $E_w = J/\omega\epsilon_0 \approx 10^6$ V/m at α-to-γ transition

He/H_2O MODELING

- In an experiment, a 1 cm radius 0.5 mm gap discharge was embedded in a large chamber with fixed H_2O concentration

(P. Bruggeman et al, JPD 43, 012003, 2010)



- In a global model (46 species, 577 reactions), particle and energy balance were solved to determine the discharge equilibrium

(D.X. Liu et al, PSST 19, 025018, 2010)

- Discharge depletes external H_2O density, reaction products diffuse to axial and radial walls, sheaths cause α-to-γ transition

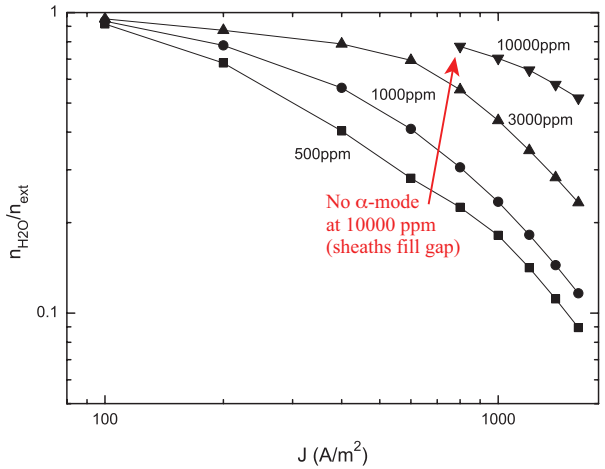
He/H_2O ADDITIONAL HYBRID MODEL PHYSICS

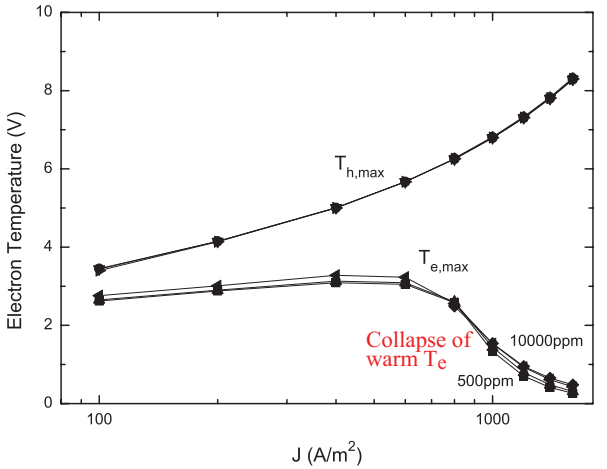
(Ke Ding et al, JPD 47, 305203, 2014)

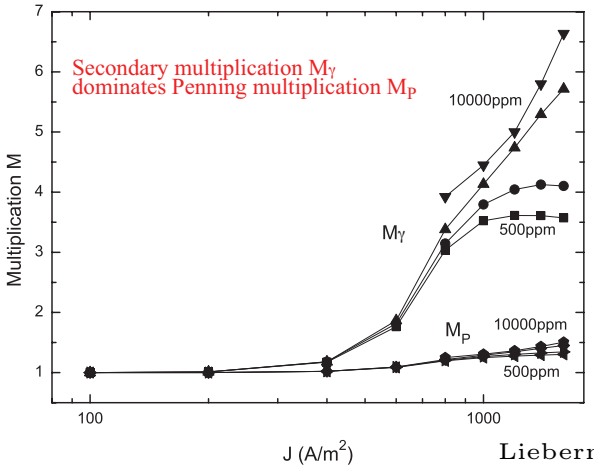
- Diffusive flow of H_2O into discharge region (analytic)
- Diffusive flow of reaction products to walls (analytic)
- Multiple Penning processes and positive ion wall losses (numerical)
- 203 reactions, 43 species (includes clusters up to $H_{19}O_9^+$)

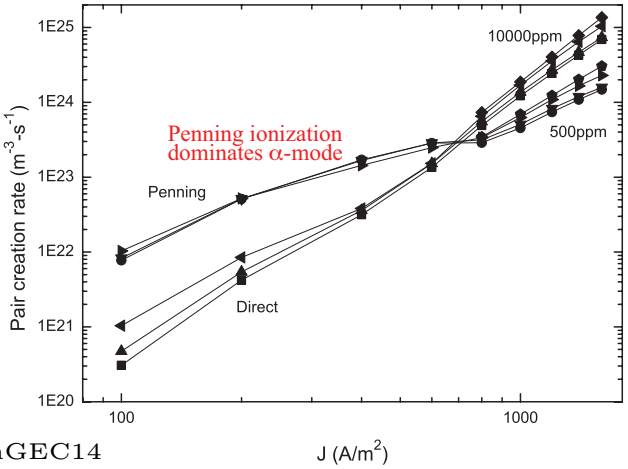
VARIATIONS WITH J AND H_2O CONCENTRATION

- Radius 1 cm, gap 0.5 mm, 13.56 MHz, secondary emission = 0.25



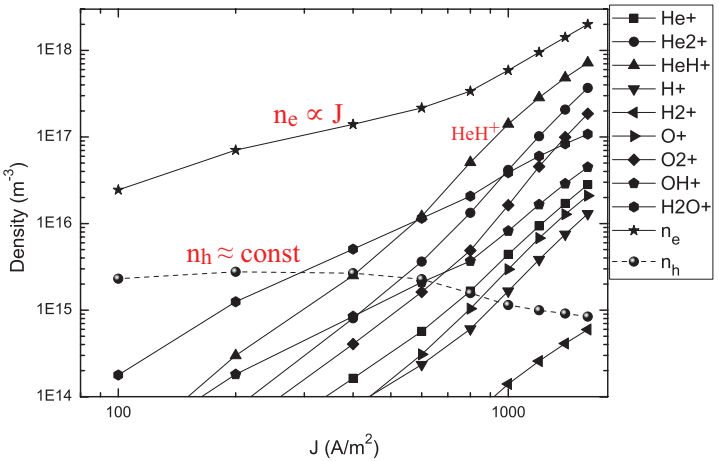


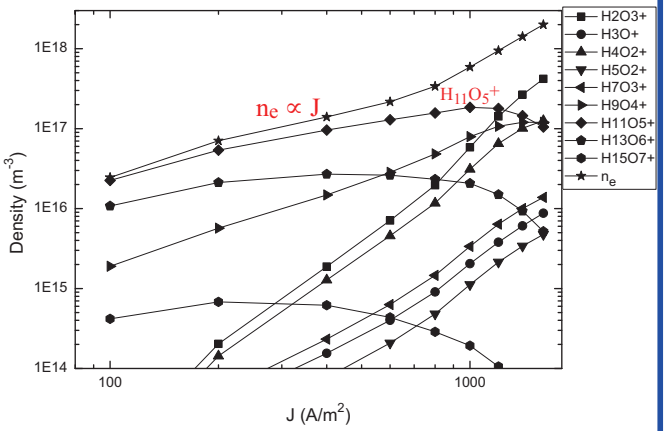




DENSITY VARIATIONS WITH J AT 1000 ppm H_2O

- Radius 1 cm, gap 0.5 mm, 13.56 MHz, secondary emission = 0.25





- $H_{11}O_5^+$ is the main ion in α-mode
- HeH^+ is the main ion in the γ-mode
- The α-mode scalings $n_e \propto J$ and $n_h \approx$ const are seen

PRINCIPAL REACTION PATHWAYS ANALYSIS

(Ke Ding et al, submitted to JPD, 2014)

- Open source software package `PumpKin` (www.pumpkin-tool.org)

  (A. H. Markosyan, A. Luque, F. Gordillo-Vazquez, and U. Ebert, Comput. Phys. Commun. 185, 2697, 2014)

- Example of O_2 formation from H_2O
  - The important intermediates are OH, HO_2, and H_2O_2
  - OH is produced from H_2O via Penning ionization-initiated cluster formation, and also by direct electron dissociation
  - OH production is followed by

$$2 \cdot (2\,OH + He \rightarrow H_2O_2 + He)$$

$$e + H_2O_2 \rightarrow 2\,OH + e$$

$$OH + H_2O_2 \rightarrow HO_2 + H_2O$$

$$OH + HO_2 \rightarrow O_2 + H_2O$$

SUMMARY

- We used PIC simulations of a He/N_2 atmospheric pressure rf capacitive discharge, with simplified chemistry, to develop a hybrid global model including sheaths and two electron temperatures.
- The hybrid model simulations of the discharge gave reasonable agreement with the PIC simulations, including the α-to-γ transition.
- We added trace gas depletion and reaction product diffusion to the hybrid model to simulate a chemically complex He/H_2O bounded discharge.
- We determined the H_2O depletion, the reaction product diffusion, the α-to-γ transition, the suppression of the α-mode by the sheaths at high H_2O concentrations, and the principal pathways for various species.

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