Capacitively and inductively coupled high frequency discharge in one and two dimensional PIC-MCC simulations

Irina Schweigert

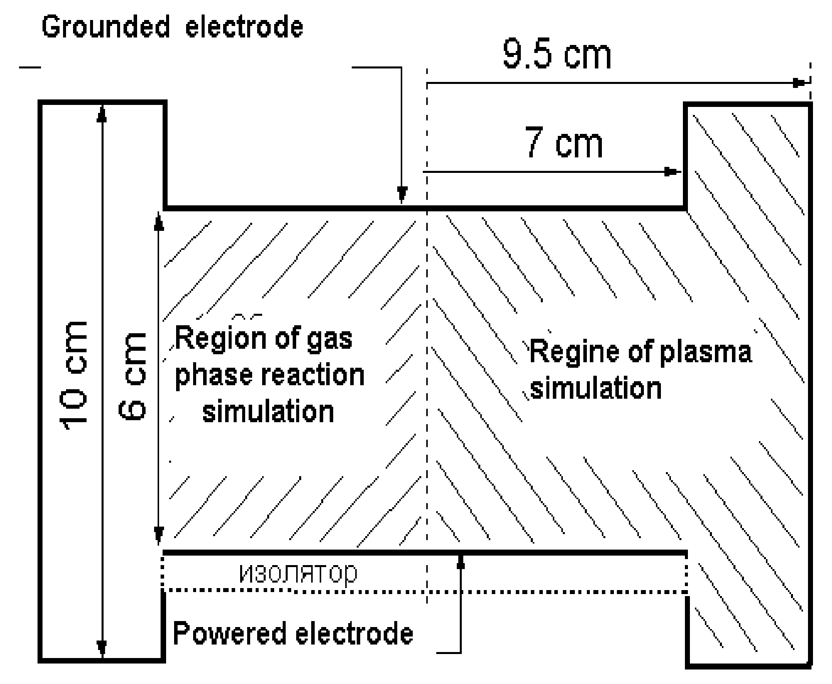
Institute of Theoretical and Applied Mechanics, SB RAS, Novosibirsk

With collaboration with
Vitaly Schweigert,
Andrey Alexandrov,
Evgeny Bondar

Outline

- (i) New combined PIC-MCC algorithm
- (ii) Different modes of ccrf discharge operation in methane
- (iii) New fast PIC-MCC algorithm
- (iv) Non - flat electrode problem
- (v) Inductively coupled planar discharge simulation

One and two dimensional simulations



Kinetic simulations of ccrf discharge in Ar, He, CH_4

$P=(0.01-1)$ Torr, $n=(10^8-10^{10})cm^{-3}$

Problem:
Artificial heating of electrons
in bulk plasma on numerical fluctuations of E

Combined model: PIC-MCC + fluid model,

I.V. Schweigert, V.A. Schweigert,
Plasma Source Sci Technol. 13, 315 (2004)

(1) $$\frac{\partial f_{e,i}}{\partial t} + \vec{v}_{e,i}\frac{\partial f_{e,i}}{\partial \vec{r}} \mp \frac{e\vec{E}}{m}\frac{\partial f_{e,i}}{\partial \vec{v}_{e,i}} = J_{e,i},$$

(2) $$\frac{\partial n'_e}{\partial t} + \frac{\partial j'_e}{\partial x} = Q, \quad \frac{\partial n'_i}{\partial t} + \frac{\partial j'_i}{\partial x} = Q,$$

(3) $$\frac{\partial j'_{e,i}}{\partial t} = -\frac{\partial T'_{e,i} n'_{e,i}}{\partial x} \mp \frac{e\vec{E}}{m} n'_{e,i} - \nu_{e,i} j'_{e,i} - Q_{e,i}$$

(4) $$\Delta\phi = 4\pi e(n'_e - n'_i), \quad E = -\frac{\partial \phi}{\partial x}.$$

$$Q = N_g \int v_{ex}\sigma_i f_e d\vec{v}_e$$

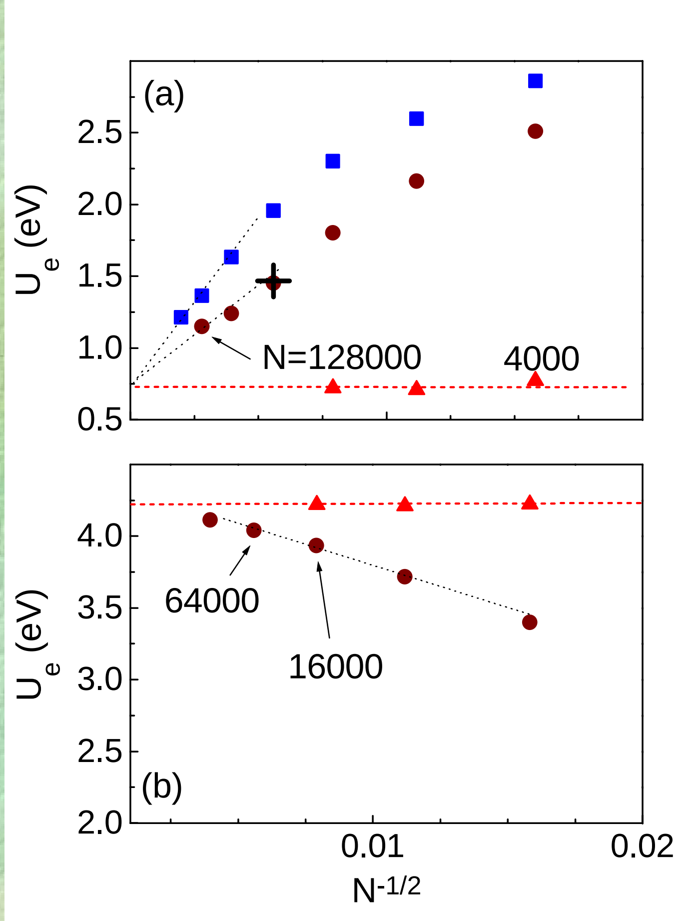
$$T'_e = \frac{\int v_{ex}^2 f_e d\vec{v}_e}{\int f_e d\vec{v}_e}, \quad T'_i = \frac{\int v_{ix}^2 f_i d\vec{v}_i}{\int f_i d\vec{v}_i}$$

$$Q_e = N_g \int v_{ex}|\vec{v}_e|\sigma_t f_e d\vec{v}_e - \nu_e \int v_{ex} f_e d\vec{v}_e,$$

$$Q_i = N_g \int v_{ix}|\vec{v}_i|\sigma_r f_i d\vec{v}_i - \nu_i \int v_{ix} f_i d\vec{v}_i$$

$$\nu_e = \frac{N_g \int |\vec{v}_e|\sigma_t f_e d\vec{v}_e}{\int f_e d\vec{v}_e}, \quad \nu_i = \frac{N_g \int |\vec{v}_i|\sigma_r f_i d\vec{v}_i}{\int f_i d\vec{v}_i},$$

Combined PIC-MCC model

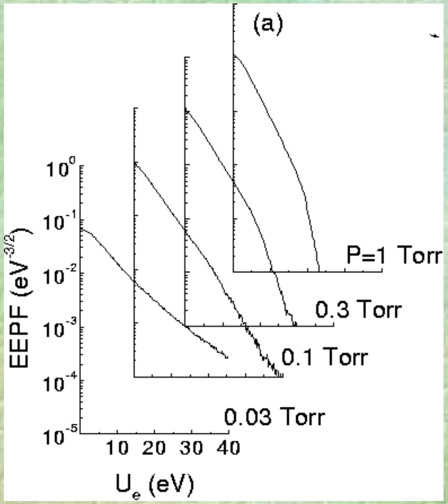


Mean electron energy from the total number of simulation particles for P=0.1Torr (a) and P=0.3Torr (b) calculated with the standard PIC-MCC method (②), with the PIC-MCC SS method (➔) with spatial smoothing of the space charge and electrical field distributions and with our combined algorithm (⇩). '⌧' Birdsall, 1991 with N=32000, d=2cm, j=2.65mA/cm2.

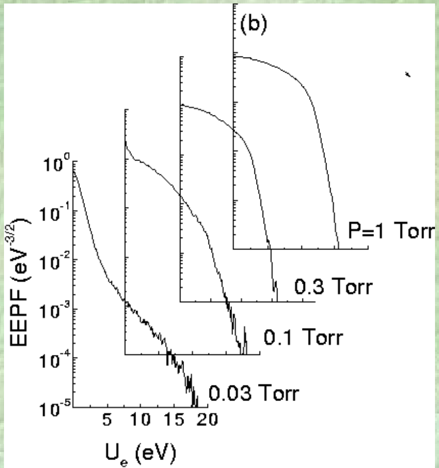
- - - - exp-t, Godyak, 1992.

Electron energy distribution function

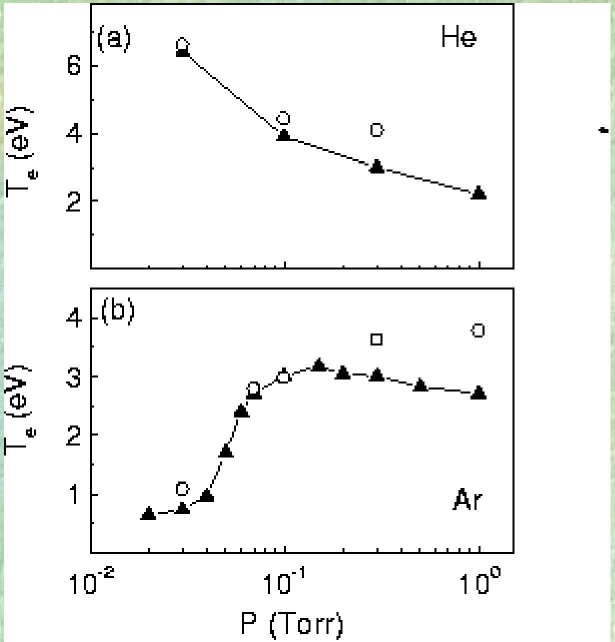
Helium

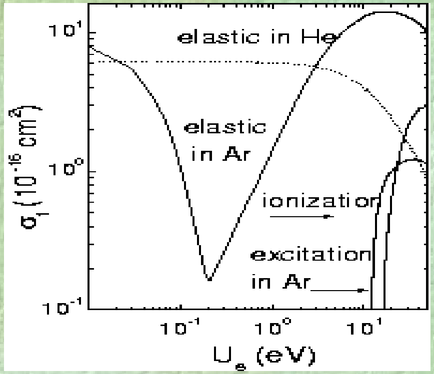


Argon



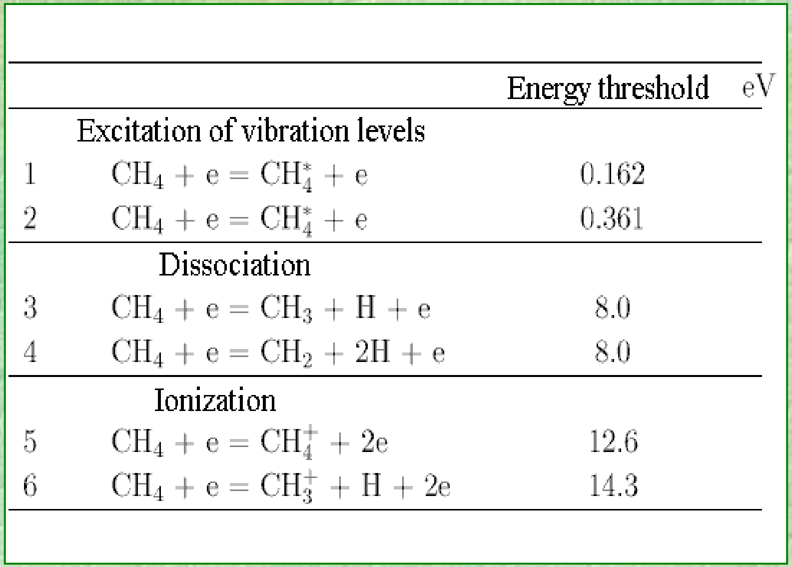
Experiment of Godyak, 1992,
d=6.7 см, j=1 мА/см^2



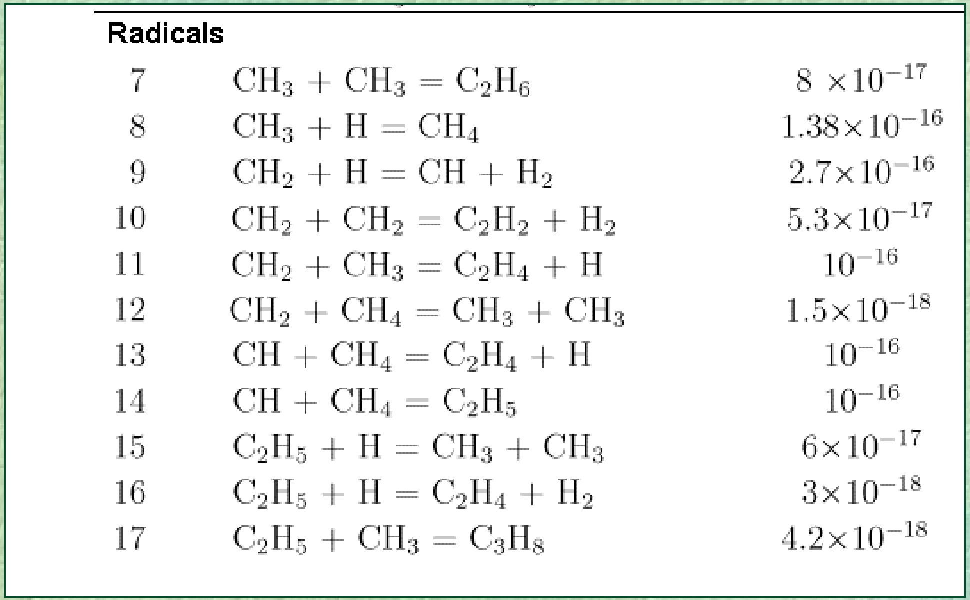


Ccrf discharge in methane

(I.V. Schweigert, Phys. Rev. Lett. 92, 55001 (2004),
I.V. Schweigert, JETP 99, 719 (2004))



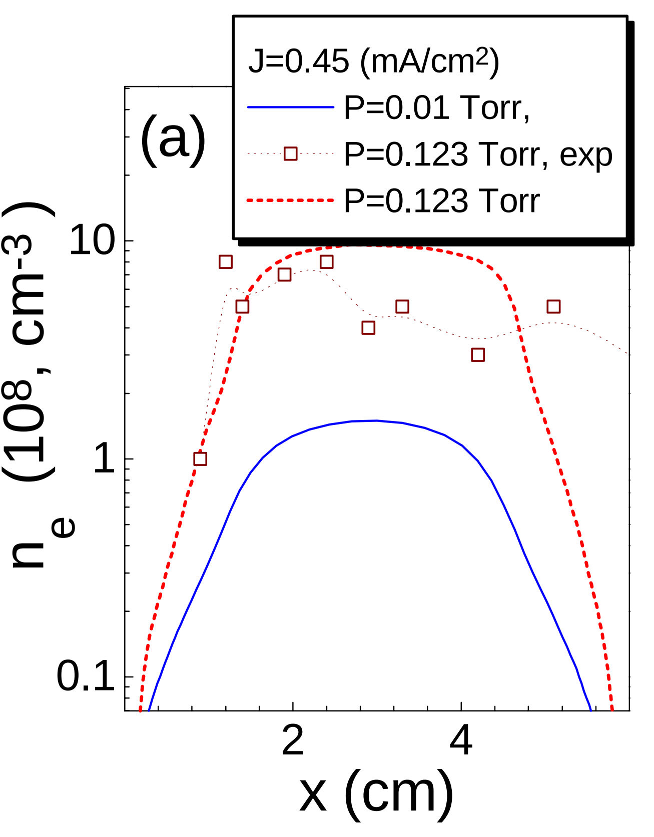
		Energy threshold eV
	Excitation of vibration levels	
1	$CH_4 + e = CH_4^* + e$	0.162
2	$CH_4 + e = CH_4^* + e$	0.361
	Dissociation	
3	$CH_4 + e = CH_3 + H + e$	8.0
4	$CH_4 + e = CH_2 + 2H + e$	8.0
	Ionization	
5	$CH_4 + e = CH_4^+ + 2e$	12.6
6	$CH_4 + e = CH_3^+ + H + 2e$	14.3



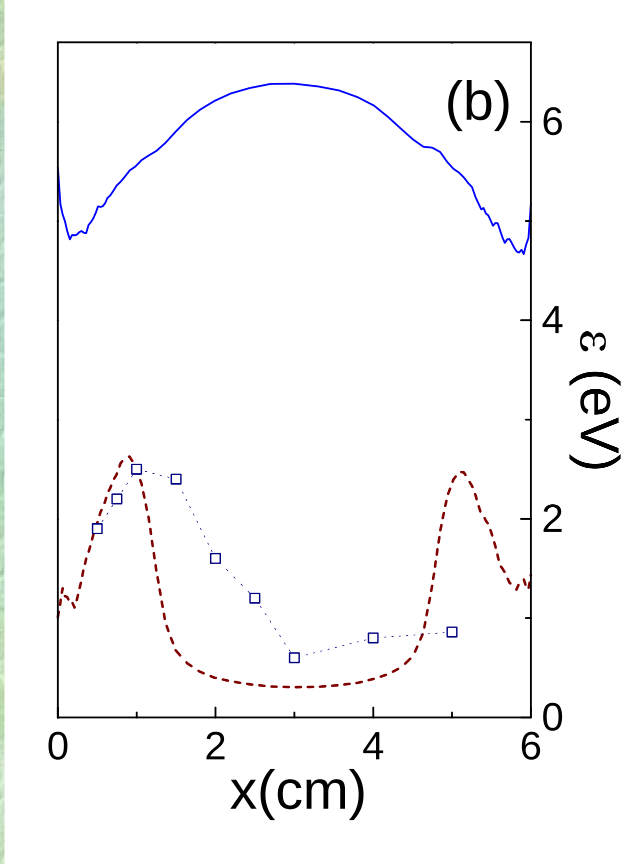
Radicals		
7	$CH_3 + CH_3 = C_2H_6$	8×10^{-17}
8	$CH_3 + H = CH_4$	1.38×10^{-16}
9	$CH_2 + H = CH + H_2$	2.7×10^{-16}
10	$CH_2 + CH_2 = C_2H_2 + H_2$	5.3×10^{-17}
11	$CH_2 + CH_3 = C_2H_4 + H$	10^{-16}
12	$CH_2 + CH_4 = CH_3 + CH_3$	1.5×10^{-18}
13	$CH + CH_4 = C_2H_4 + H$	10^{-16}
14	$CH + CH_4 = C_2H_5$	10^{-16}
15	$C_2H_5 + H = CH_3 + CH_3$	6×10^{-17}
16	$C_2H_5 + H = C_2H_4 + H_2$	3×10^{-18}
17	$C_2H_5 + CH_3 = C_3H_8$	4.2×10^{-18}

Two modes of discharge operation

Electron density



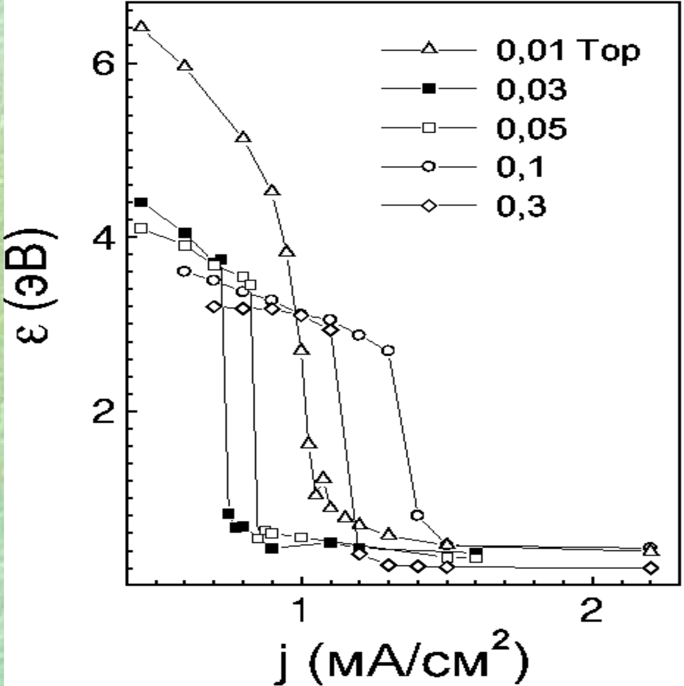
Electron energy



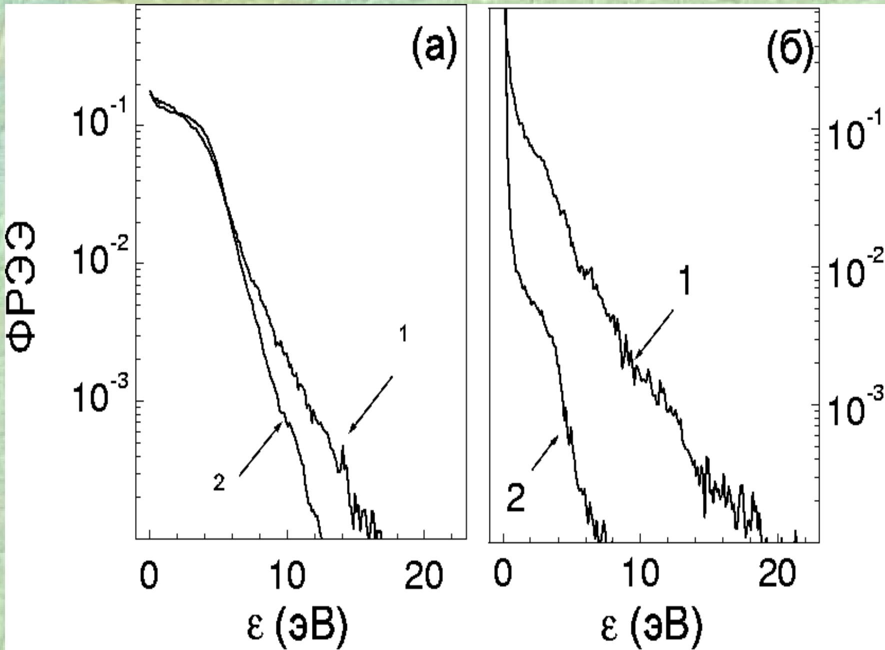
symbols – Sugai, exp. 1990

Electron energy at the transition between different modes of ccrf discharge

Electron energy distribution function



Mean electron energy in the center of discharge. Role of secondary electrons are negligible.



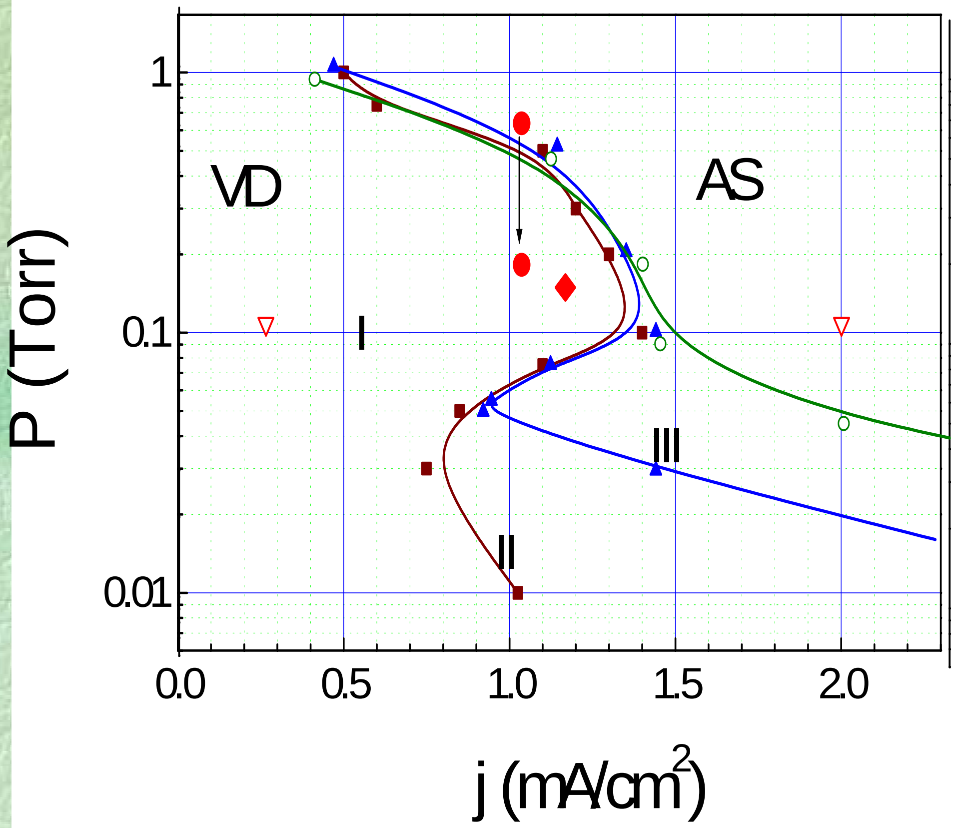
(a) VD (j=1mA/cm^2),

(b) AS (j=1,1mA/cm^2)

1 – at sheath, 2 – in center,

P=0,075Торр и d=6см

Diagram of rf discharge modes in methane



Links :

⬁Ivanov *at el*, J. Appl. Phys. 2002

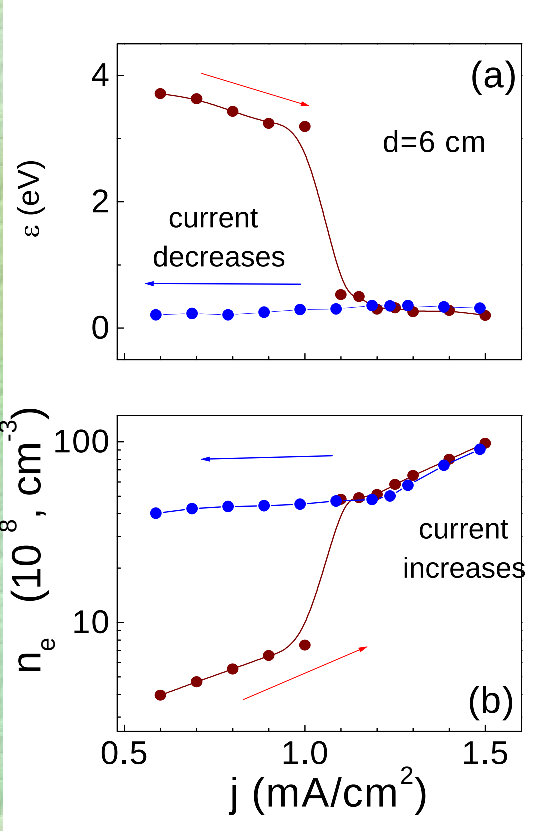
➔Bera *et al*, Plasma

- **Source Sci Technol.,**
- **2001**

➚Nagayama *et al*,

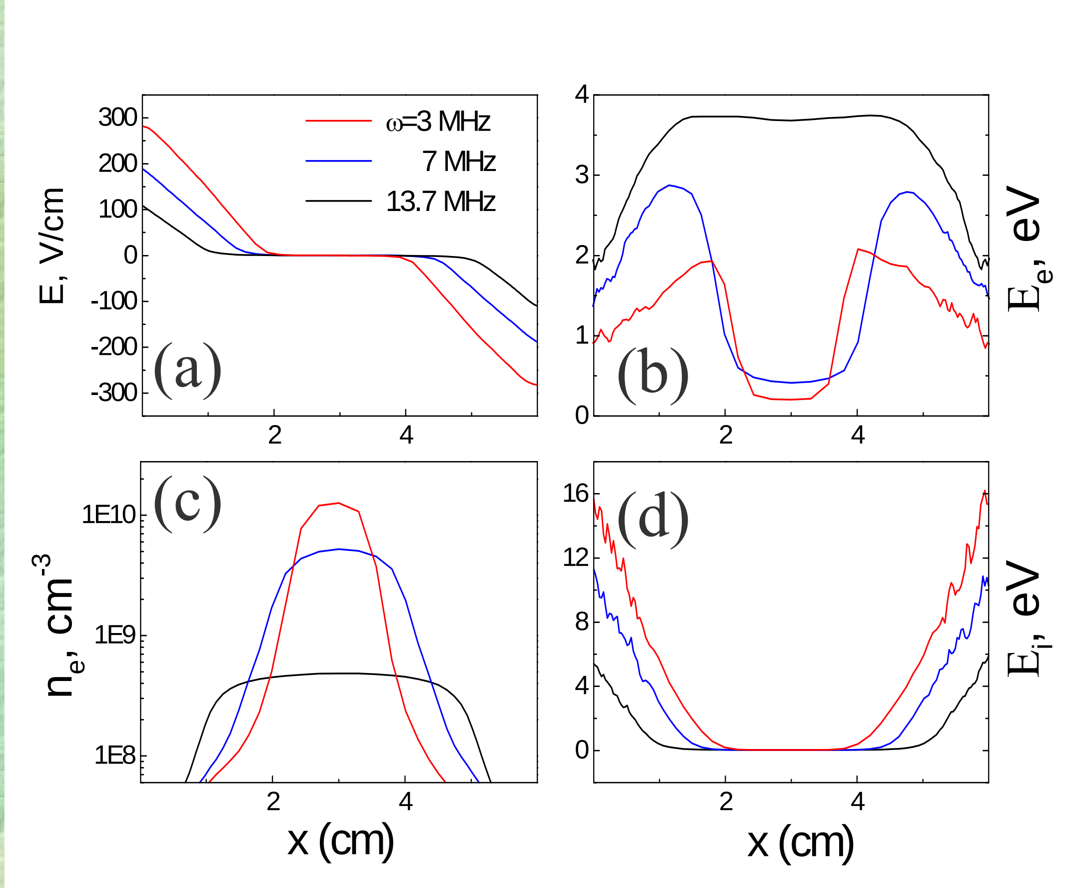
- **IEEE Trans on Plasma.**
- **Science 1998**

Hysteresis in ccrf discharge in methane



Hysteresis was observed
C. Bohm and J. Perrin
J. Phys. D: Appl.
Phys. (1991)
in the silane discharge.

Impact of discharge frequency on plasma parameters



- j=0.5 mA/cm2, d=6 cm, P=0.075 Torr electrical field (a) electron density (b) electron energy (c)
- mean ion energy (d) for discharge frequencies
- 13.7 MHz —
- 7 MHz —
- 3 MHz —

Two dimensional fast PIC-MCC approach

(I.V. Schweigert, A.Alexandrov, IEEE Trans. on Plasma Science 32, 615 (2005),

A.Alexandrov, I.V. Schweigert, Plasma Sources Sci. Technol. 14, 209 (2005))

1 step

$$\frac{\partial f_i}{\partial t} + \vec{v}\frac{\partial f_i}{\partial \vec{r}} + \frac{eZ_i\vec{E}}{m_i}\frac{\partial f_i}{\partial \vec{v}} = J_i, \qquad (1)$$

$$\frac{\partial f_e}{\partial t} + \vec{v}\frac{\partial f_e}{\partial \vec{r}} - \frac{e\vec{E}}{m_e}\frac{\partial f_e}{\partial \vec{v}} = J_e, \qquad (2)$$

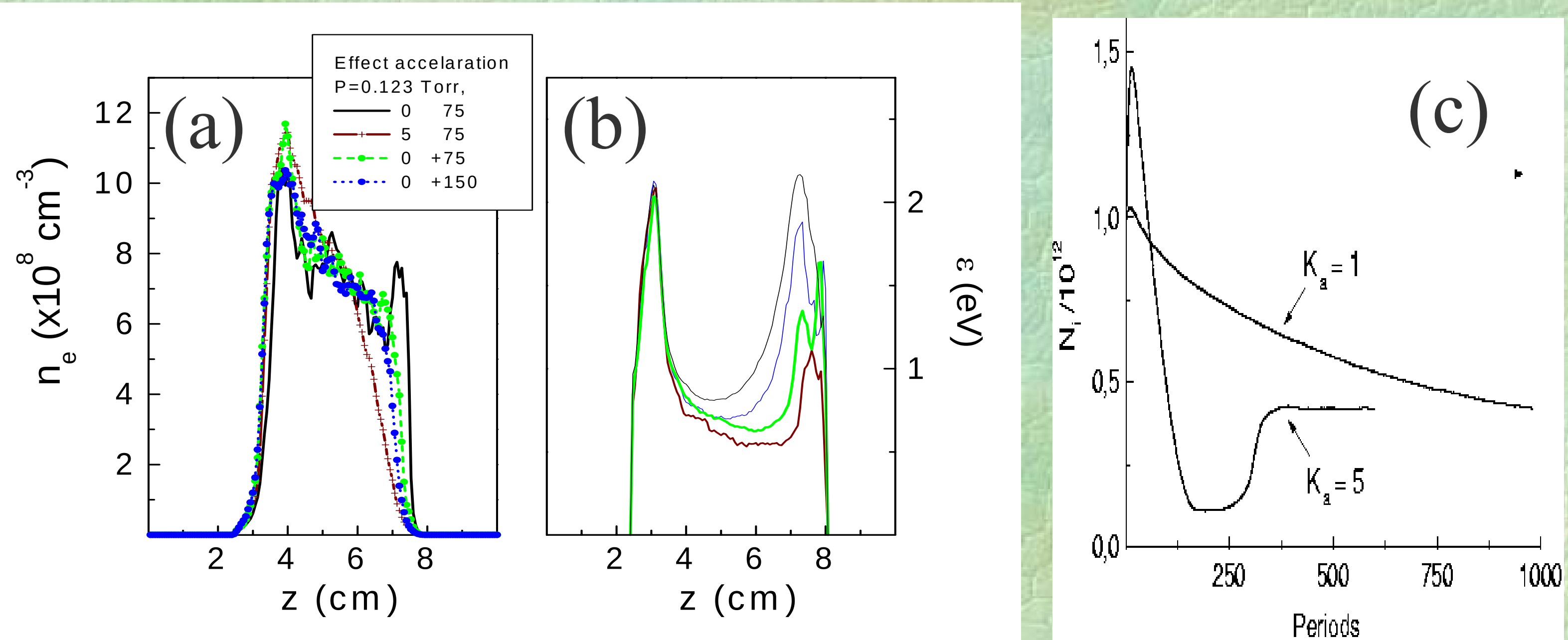
$$\triangle\phi = 4\pi e(n_e - \sum_i Z_i n_i), \quad \vec{E} = -\frac{\partial \phi}{\partial \vec{r}}. \qquad (3)$$

2 step

$$\frac{\partial f_i}{\partial t} + \vec{v}\frac{\partial f_i}{\partial \vec{r}} + \frac{eZ_i\vec{E}_a}{m_i}\frac{\partial f_i}{\partial \vec{v}} = J_i \equiv J_{i,1} + J_{i,2}, \qquad (4)$$

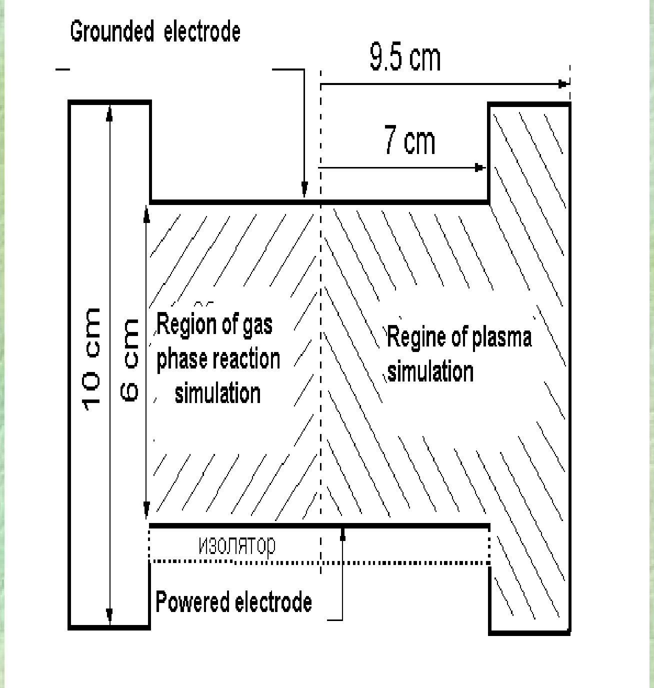
$$\vec{E}_a = <\vec{E}> - \frac{\vec{\nabla} T_e n_{ia}}{n_{ia}} + \frac{\vec{\nabla} T_e n_i}{n_i}, \qquad (6)$$

Two dimensional fast PIC-MCC simulations. Acceleration effect.

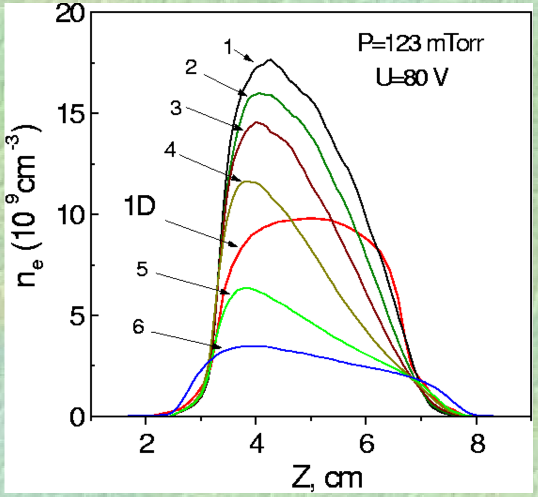


Relaxation of electron density (a), electron energy (b) and total ions number (c) during PIC-MCC simulation for acceleration factor K_a=5 and without acceleration K_a=1

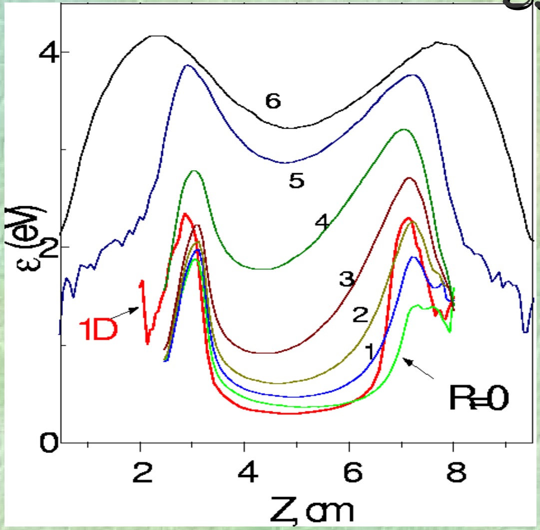
Comparison of 1D and 2D results



Electron density

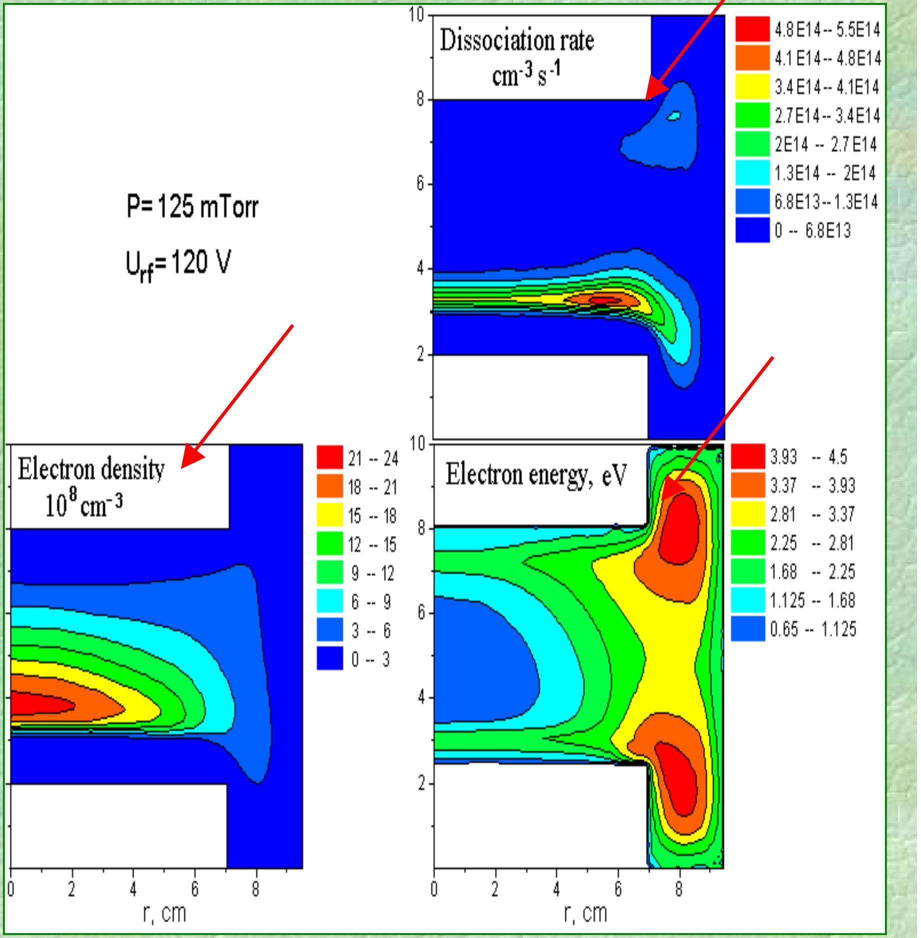


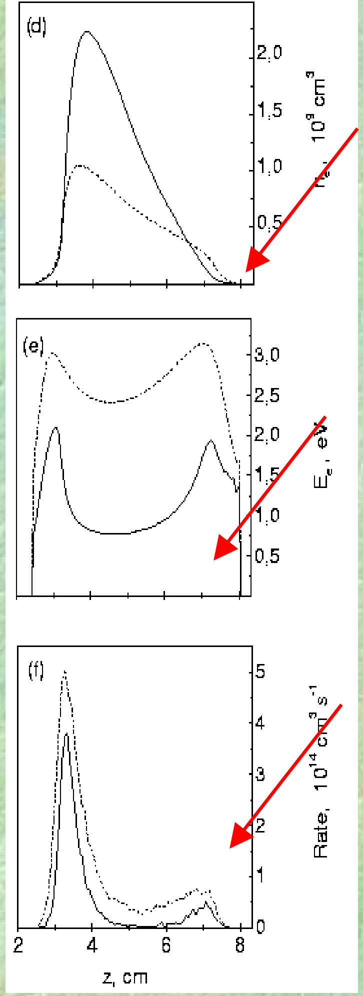
Mean electron energy



R=0 - 6 cm are distances from the centre of discharge chamber

2D distributions of plasma parameters in active sheath mode, P=125 mTorr, U=120 V





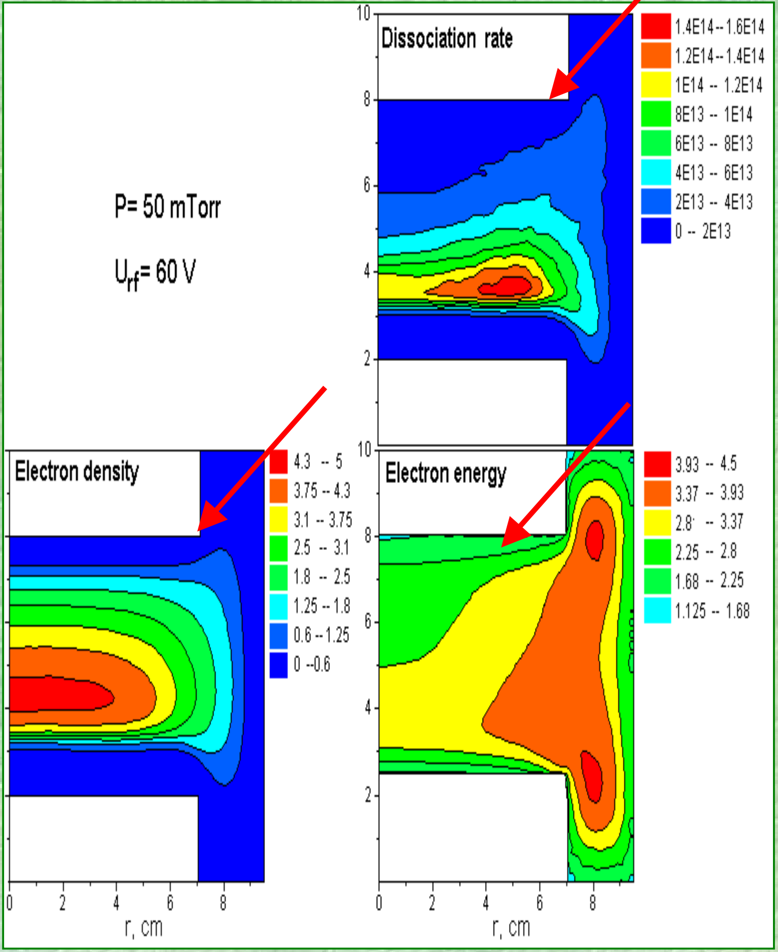
Electron density

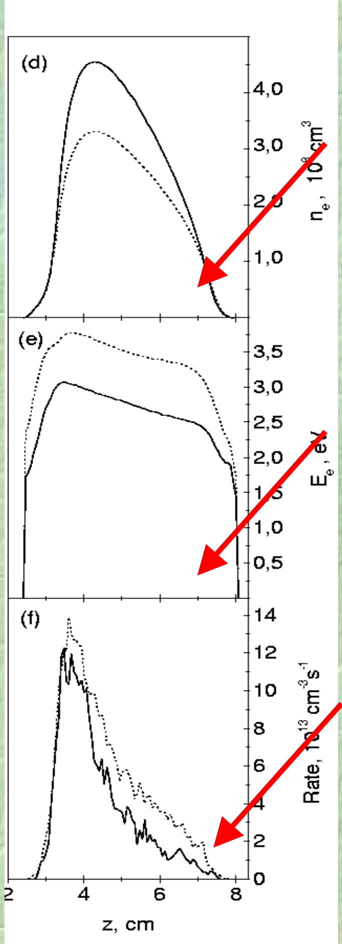
Energy of electrons

$CH_4 \rightarrow CH_3 + H$ dissociation rate

Solid lines: r = 0, dotted r = 6 cm

2D distributions of plasma parameters in volume dominated mode, P=50 mTorr, U=60 V



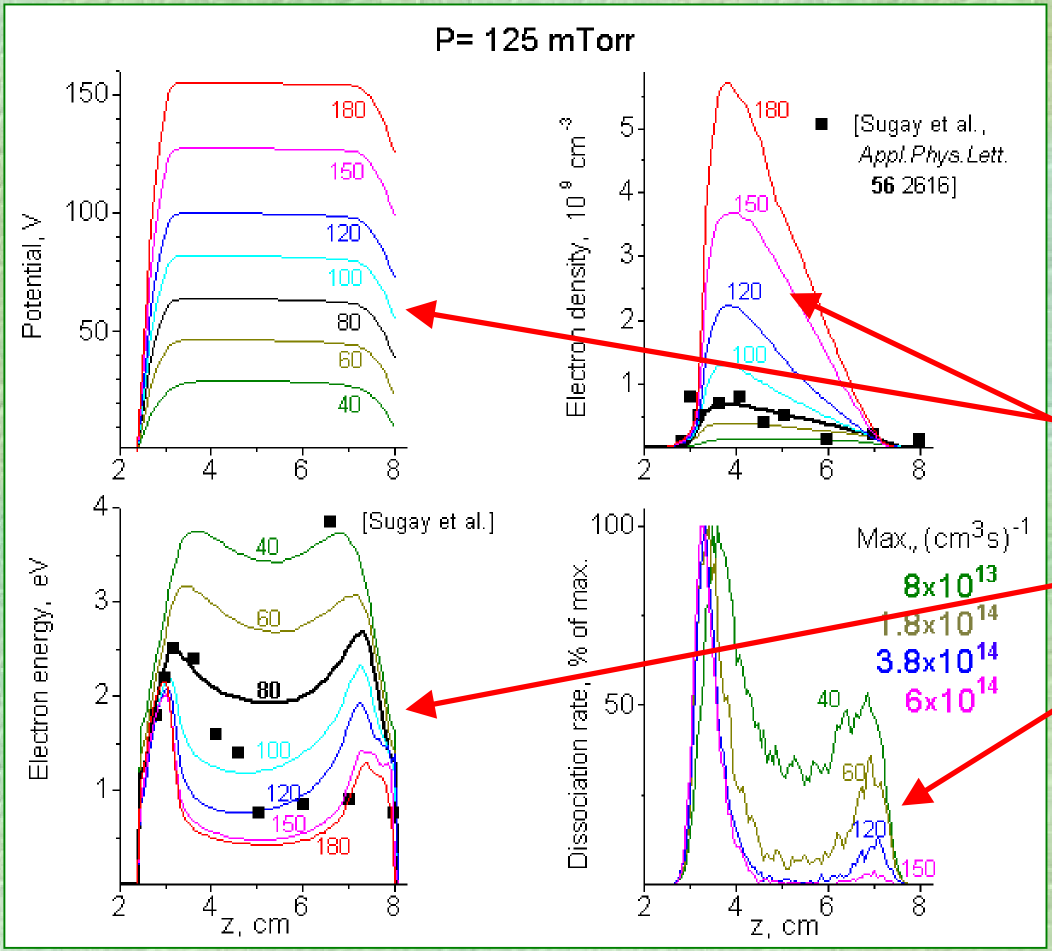


Electron density

Electron energy

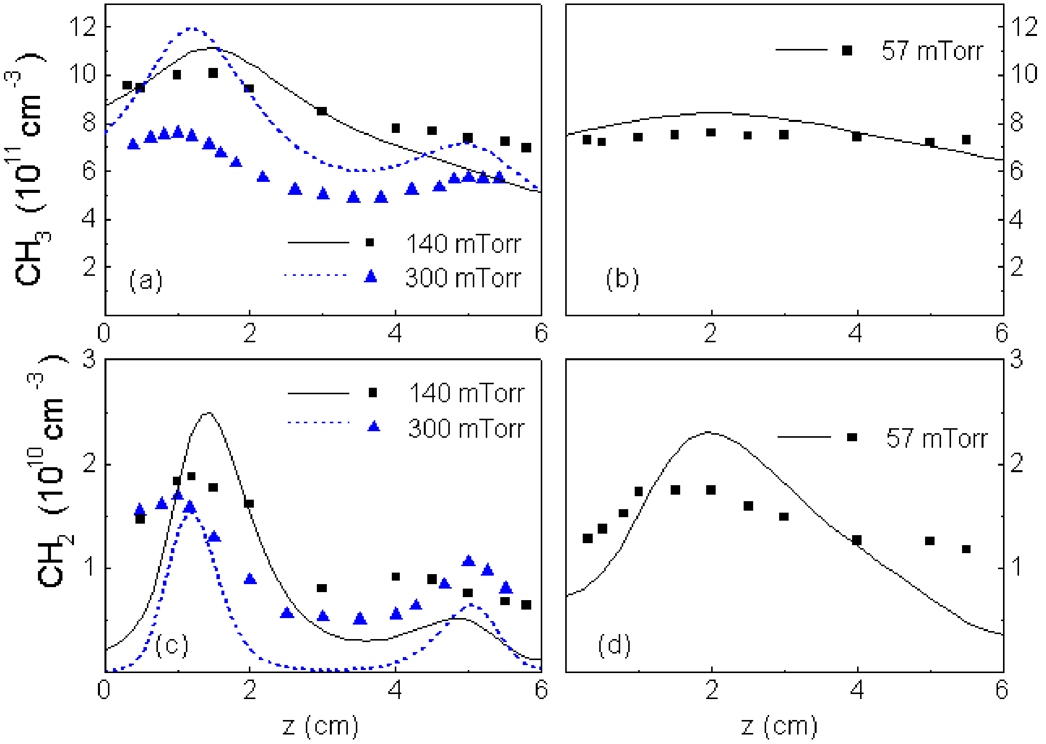
$CH_4 \rightarrow CH_3 + H$ dissociation rate

Transition between different modes in plasma reactor for P=125 mTorr



Period averaged
plasma potential,
electron density,
electron energy,
CH3+H rate for
U_{rf}=40 - 180 V.
"②" exp-t **Sugai, 1990**

Radical density distributions



Radical density, comparison with experiments

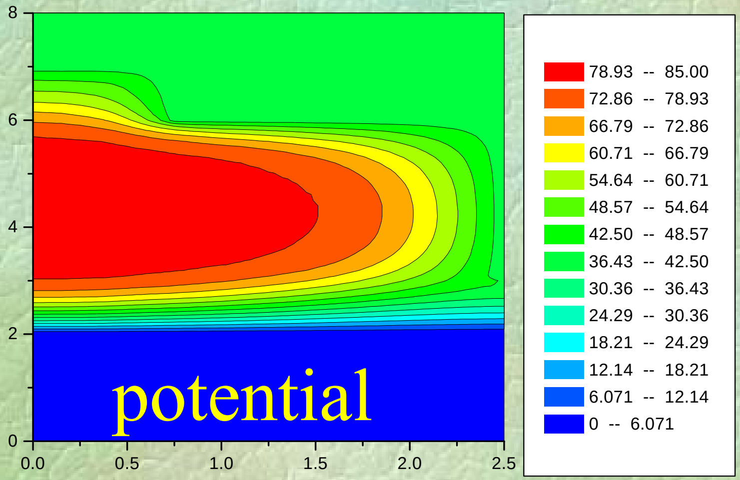
(Sugai and Toyoda *J.Vac.Sci.Technol.* **A10,** 1193)

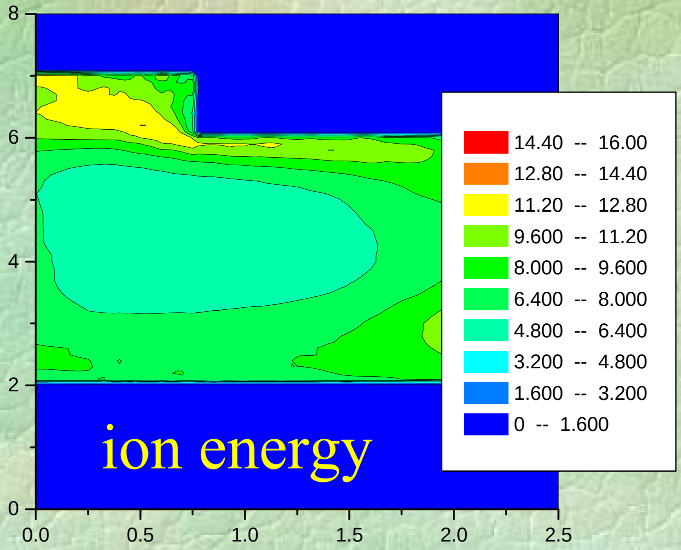
Non-flat electrode problem

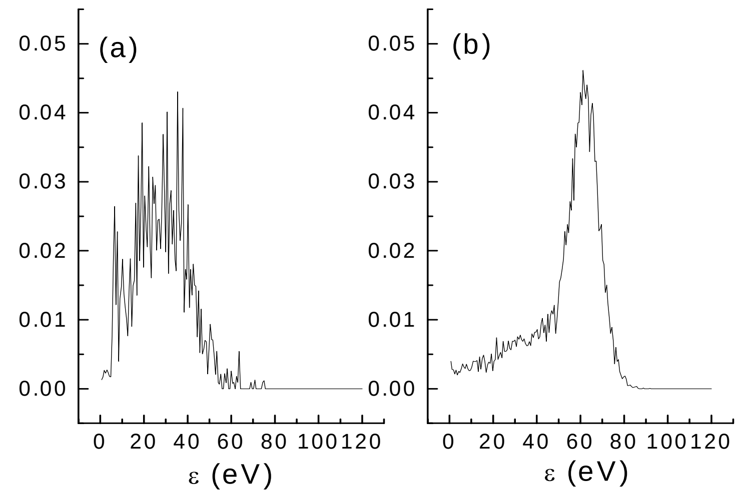
Ar, d = 4 cm, h=8 cm, R_0=2.5 cm

P=5 mTorr, U_{rf}=90 V, h_c=1cm

The ion energy distribution function on cavity bottom (a) on flat electrode (b)

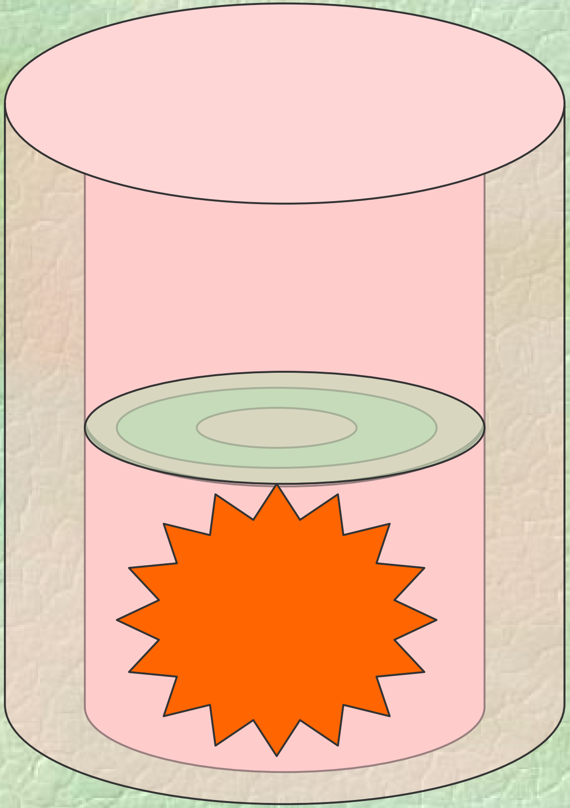






- Summary
- The efficient algorithms for kinetic simulation of ccrf gas discharge are developed. The results have been published in recent papers:
- - V.A. Schweigert, A.L. Alexandrov, S.F. Gimelshein and M.S. Ivanov,
  PSST, 9 (1), B1-B3 (2000)
- - I.V. Schweigert, V.A. Schweigert,
  Plasma Source Sci Technol. 13, 315 (2004)
- - I.V. Schweigert, Phys. Rev. Lett. 92, 55001 (2004).
- - I.V. Schweigert, JETP 99, 719 (2004).
- - A.Alexandrov, I.V. Schweigert, Plasma Sources Sci. Technol. 14, 209 (2005).
- - I.V. Schweigert, A.Alexandrov, IEEE Trans. on Plasma Science 32, 615 (2005).

Particle-in-Cell Monte-Carlo modeling of planar inductively coupled discharge



typical parameters:

- gas (Ar) pressure P=0.05-13.3 Pa
- driving frequency f=3.39-21.1MHz
- discharge power 6-200 W
- discharge volume 3000 cm^3
- plasma density 10^{10}-10^{12} cm^{-3}
- gas temperature 300-500K

ICP model : main assumptions

We use:

*electron Debye length << than other relevant lengths:
quasineutrality ($n_e=n_i$) with Bohm ion velocity at the walls

*energy and density relaxation time >> discharge period:
electron distribution over energy is steady state

***ground state ionization by electron impact and plasma decay at the walls**

*wave length >> discharge size: **reduced Maxwell equations**

We don’t use:

** two-term approximation for electron distribution*

**fluid approach for ions*

**only the electric field E_θ influences the electron motion*

**only the main harmonic of solenoidal electric field is considered*

**gas density and temperature are constant*

Kinetic equations for electrons with ee-collisions:

$$\frac{\partial f_e}{\partial t} + \vec{v}\,\frac{\partial f_e}{\partial \vec{r}} - \frac{e}{m}(\vec{E} + [\vec{v}\vec{H}]/c)\frac{\partial f_e}{\partial \vec{v}} = St_{ea} + St_{ee,}$$

Kinetic equation for ions to find their “effective” mobility:

$$\vec{v}\,\frac{\partial f_i}{\partial \vec{r}} + \frac{e}{M}\vec{E}_a\,\frac{\partial f_i}{\partial \vec{v}} = St_{ia} + Q_,$$

Transport equation for ions to find electric potential:

$$-div(\mu_{eff}\, n_e \vec{\nabla}\phi) = Q_{ionization}, n_e = \int f_e d\vec{v}$$

Maxwell equation for the vector potential:

$$-\Delta\vec{A} = -e\int \vec{v} f_e d\vec{v} + \vec{e}_\vartheta\, j_{coil},$$

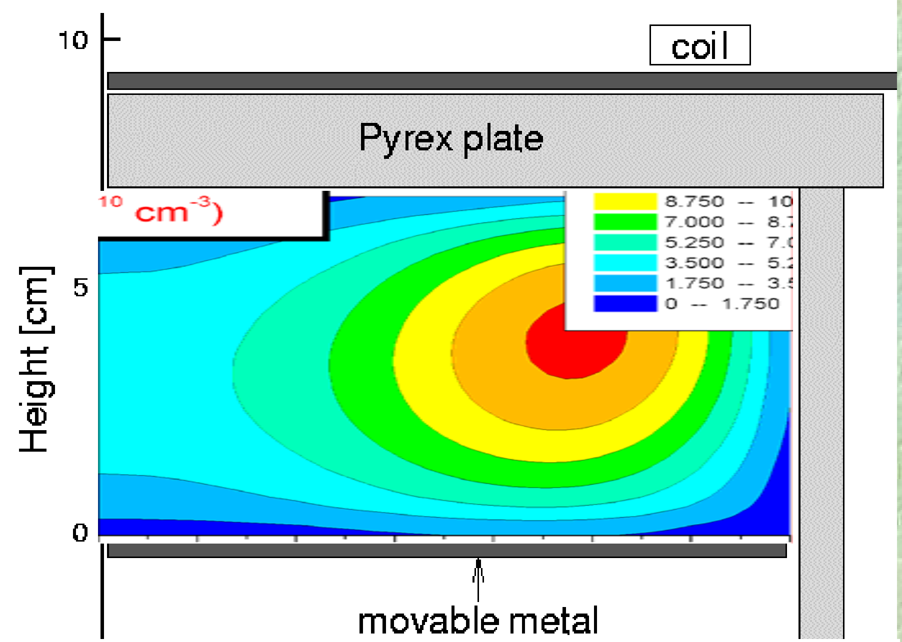
$$\vec{E} = \vec{E}_a - \frac{1}{c}\frac{\partial \vec{A}}{\partial t}, \vec{H} = rot\vec{A}, \vec{E}_a = -\vec{\nabla}\phi, \vec{A} = (A_r, A_z, A_\vartheta)$$

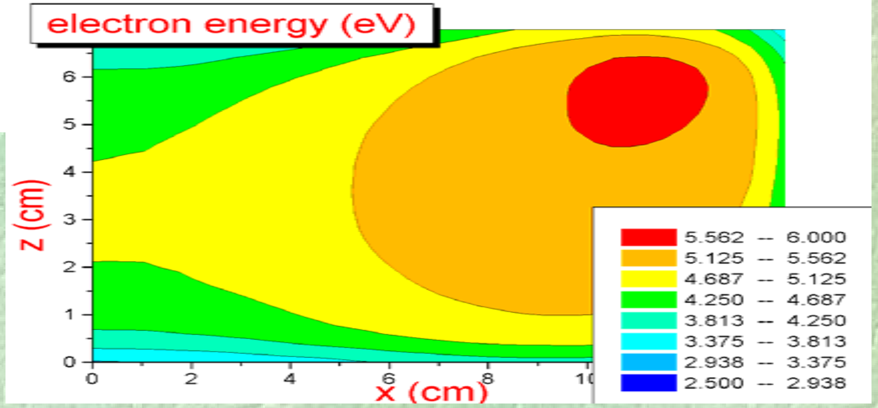
Heat conductivity to find gas temperature and density:

$$-div(\kappa\vec{\nabla}T_g) = Q_{heating}, NT_g = const$$

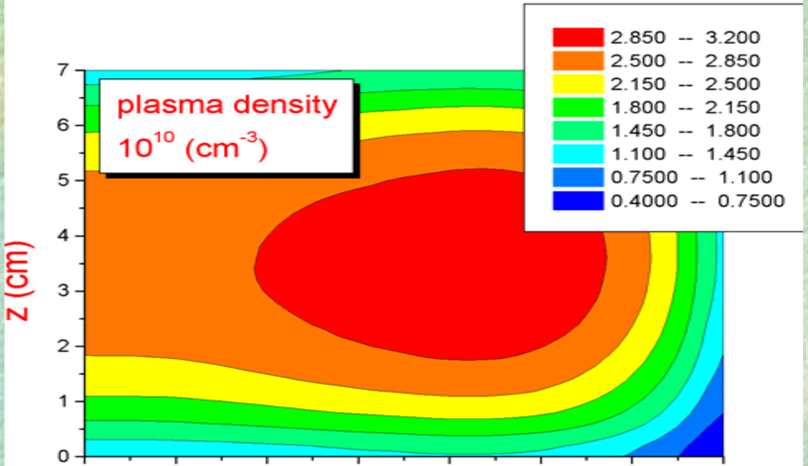
Some results of calculations

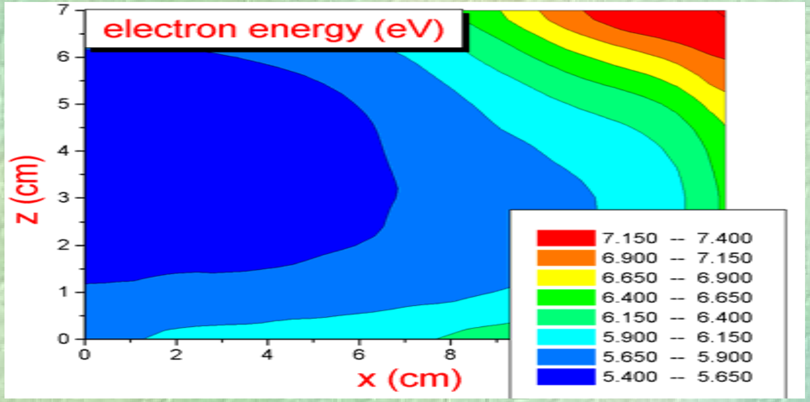
Argon pressure 2.54 Pa, power 130W





0.4Pa, power 64W





Summary

PIC/MCC model of a quasineutral, inductively plasma is developed and applied for simulations of planar inductively coupled discharge with frequency 13.56MHz and argon pressures 0.4-2.53 Pa