Comprehensive PIC-MCC model for planar sputtering magnetron discharges

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Motivation

Fluid (hybrid) description:

Heavy assumptions about:

- Transport coefficients
- Electron and ion temperature

Not necessarily valid at low pressures

Complicated equations when magnetic field is not constant

PIC/MCC

No assumption are needed

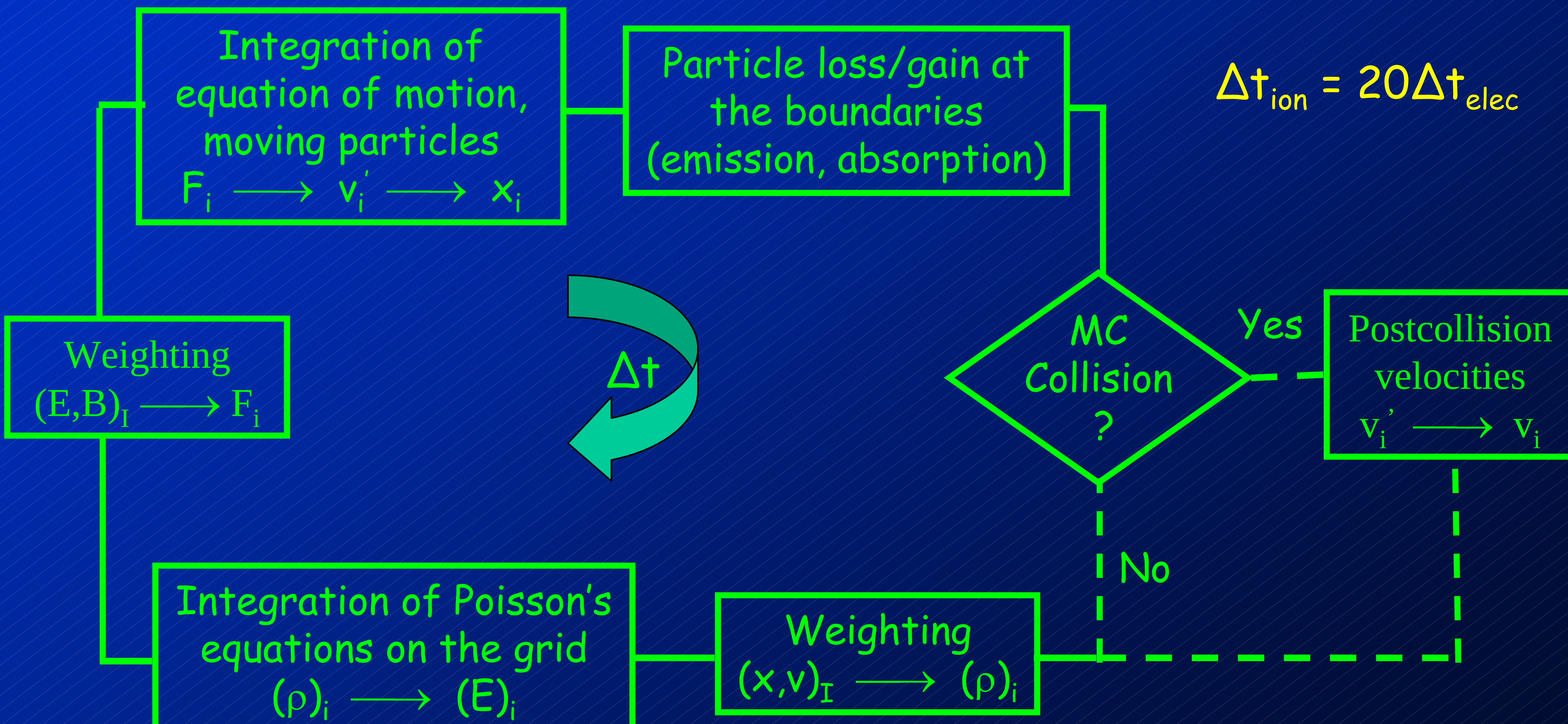
Based on first principles

Provides all the information about simulated particles

Deals with low pressures

Real Plasma Particles Replaced by Superparticles

Each superparticle represents W real particles. W is weight.



Poisson's equation (r,z)

Solved by means of Cyclic reduction method.

Swartztrauber, 1974

The potential in the discharge – superposition:

$$\phi = \phi_P + V_d \phi_L$$

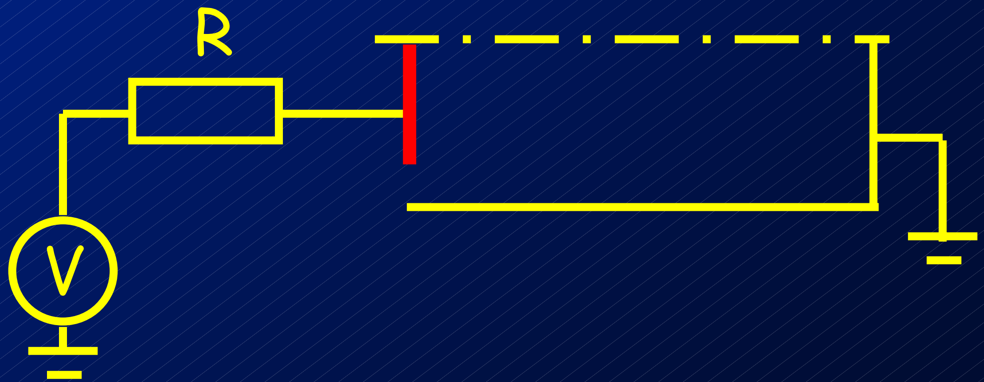
ϕ_P - solution of Poissons eq. with zero BC

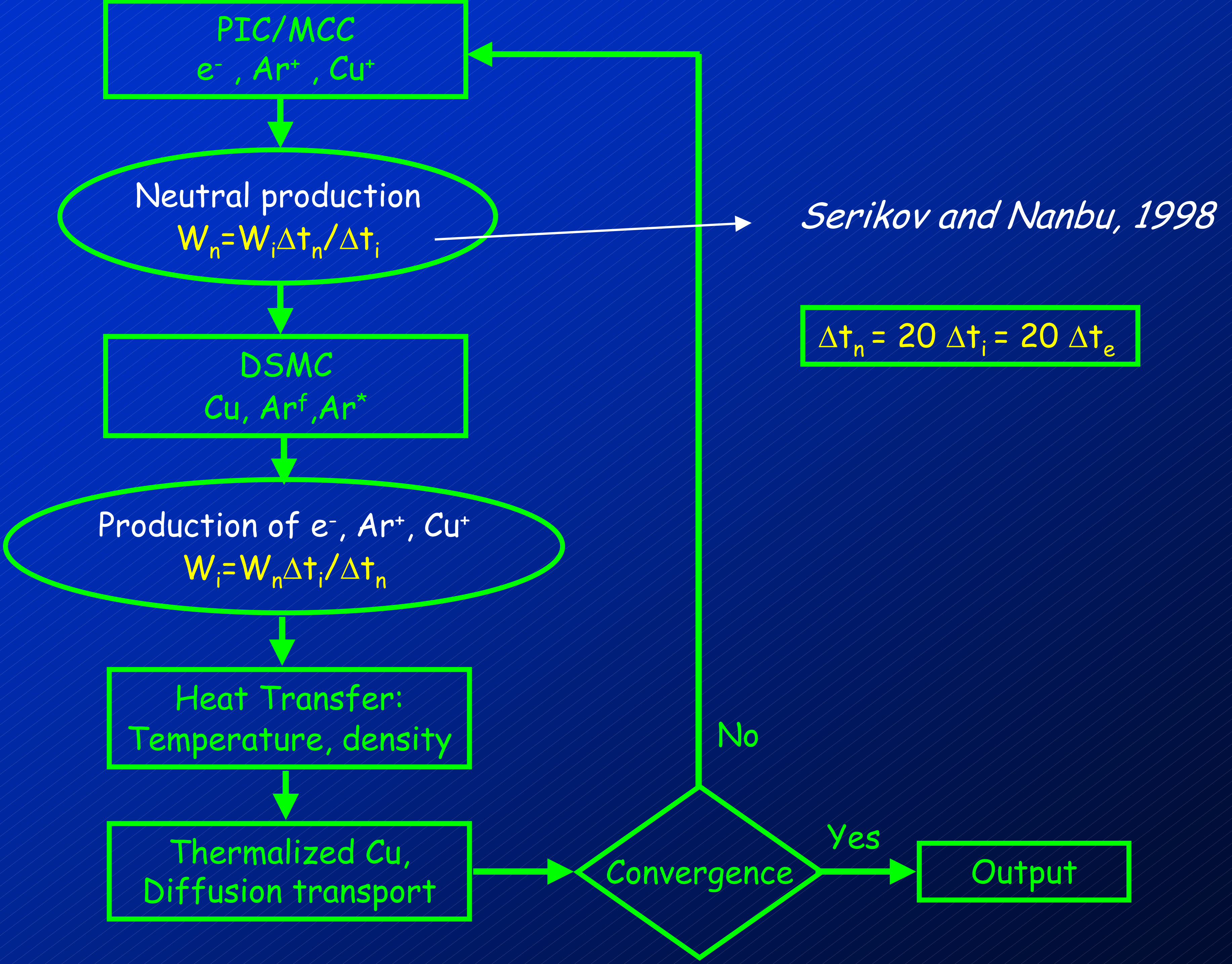
ϕ_L - solution of Laplass eq. with 1V BC on the cathode

V_d – Cathode potential, as a solution of external circuit

External circuit

Vahedi and DiPeso, 1996




PIC/MCC
e^- , Ar^+ , Cu^+
Neutral production
$W_n=W_i\Delta t_n/\Delta t_i$
Serikov and Nanbu, 1998
$\Delta t_n = 20\ \Delta t_i = 20\ \Delta t_e$
DSMC
Cu, Ar^f, Ar^*
Production of e^-, Ar^+, Cu^+
$W_i=W_n\Delta t_i/\Delta t_n$
Heat Transfer:
Temperature, density
Thermalized Cu,
Diffusion transport
No
Convergence
Yes
Output

Heat Transfer

Heat conduction equation:

$$\Delta T = -\frac{1}{k} \sum_{coll} P$$

Power imput:

$$P = \frac{m_{Ar} W_n}{V \Delta t_n} \left[\sum_k \frac{v_k'^2 - v_k^2}{2} - \sum_k{}' \frac{v_k^2}{2} + \sum_k{}^n \frac{v_k'^2}{2} \right]$$

Diffusion Transport of Cu Atoms

Diffusion equation: $$D_{Cu}\Delta n_{Cu} = r_{loss}\left(r,z\right) - r_{prod}\left(r,z\right)$$

$$r_{prod} = t\text{hermalization rate } Cu^{f}$$

$$r_{loss} = \text{rate Penning ionization} +$$
$$\text{rate electron impact ionization} +$$
$$\text{rate charge exchange between } Ar^{+} \text{ and } Cu$$

Boundary condition: $$n_{wall} = 0$$

Production and loss of Ar^m

Production processes:

$$Ar + e^- \rightarrow Ar^m + e^-$$

$$Ar + Ar^+ \rightarrow Ar^m + Ar^+$$

$$Ar + Ar^f \rightarrow Ar^m + Ar^f$$

$$Ar^+ + e^- \rightarrow Ar^m + h\nu$$

Loss processes

$$Ar^m + e^- \rightarrow Ar^+ + 2e^-$$

$$Ar^m + e^- \rightarrow Ar^* + e^-$$

$$Ar^m + Ar^m \rightarrow Ar^+ + Ar + e^-$$

$$Ar^m + e^- \rightarrow Ar^* + e^-$$

$$Ar^m + Cu \rightarrow Ar + Cu^+ + e^-$$

$$Ar^m + Ar \rightarrow Ar + Ar$$

Sputtering yield

Sputtering yield: $$Y(\varepsilon_i) = 0.42 \frac{\alpha Q K_s s_n(\varepsilon_i)}{U_s\left(1+0.35 U_s s_e(\varepsilon_i)\right)} \left[1-\left(E_{th}/E\right)^{1/2}\right]^{2.8}$$

Initial Energy: $$E_{Cu_{init}} = \frac{\sqrt{RN}}{\left(1-\sqrt{RN}\right)} U_s$$

Angular distribution: $$\theta = \frac{1}{2} \arccos\left(1 - 2RN\right)$$

Matsunami et al, 1984

RN – random number
$RN \in [0,1]$

E – incident ion/atom energy
Us – target sublimation energy

$e^- \rightarrow$ Ar collisions:

Ionization:

Opal, 1971

$$\varepsilon_{ejected} = B(\varepsilon')\tan\left[\frac{\varepsilon' - \Delta\varepsilon_{ionization}}{2B(\varepsilon')}\right]$$

$$\varepsilon_{primary} = \varepsilon' - \Delta\varepsilon_{ionization} - \varepsilon_{ejected}$$

Scattering:

$$\varepsilon'' = \varepsilon'\left(1 - \frac{2m_{e^-}}{M_{Ar^-}}(1-\cos\chi)\right)$$

Excitation:

$$\varepsilon'' = \varepsilon' - \Delta\varepsilon_{excitation}$$

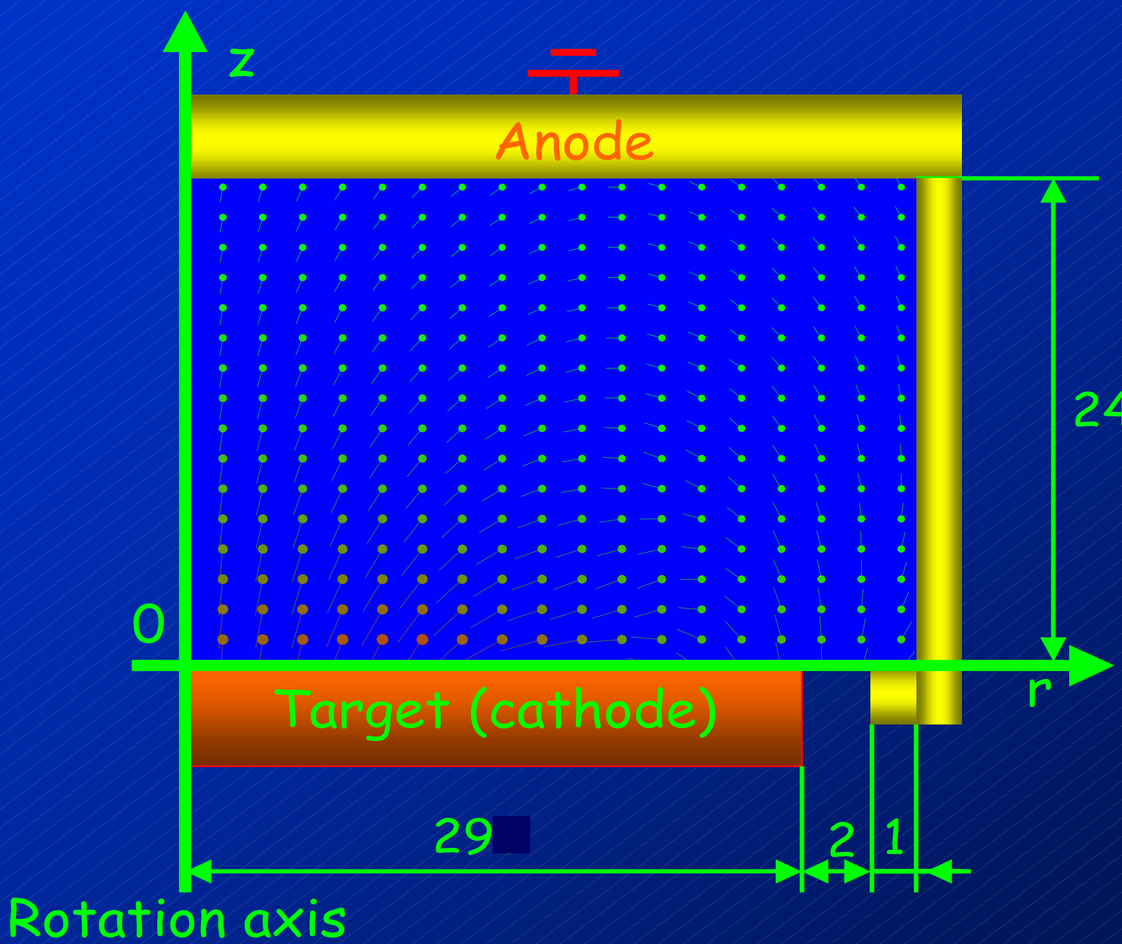
Scattering angle:

Ochrymovskii, *2002*

$$\chi = \arccos\left(1 - 2\frac{RN}{1+8E(1-RN)}\right)$$

$$E = \varepsilon_e / E_0$$

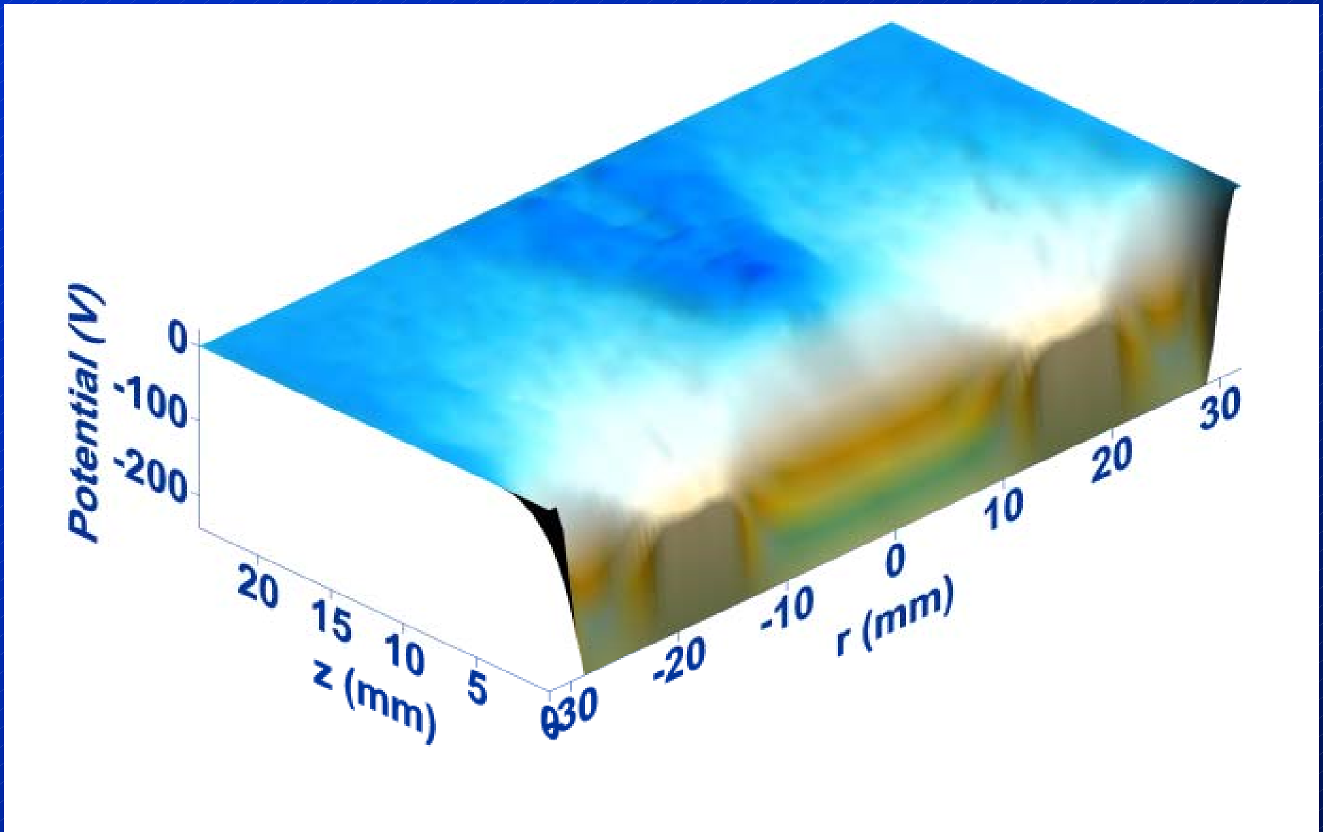
Dimensions of the Modeled System



Br_{max} = 1200 G

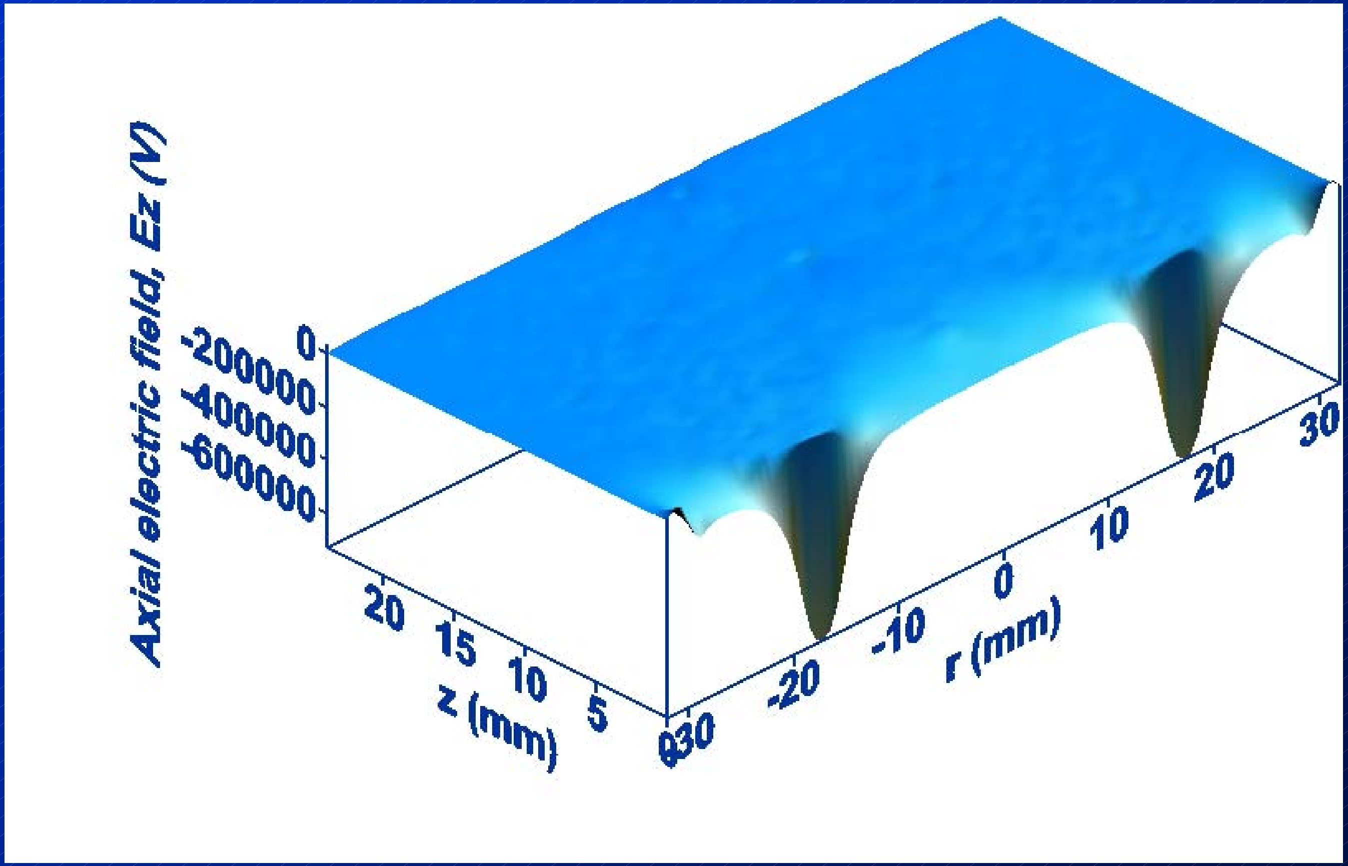
V_{ext} = -800 V
R_{ext} = 1200 Ω
p = 5 mtorr
Argon

Calculated Electric Potential

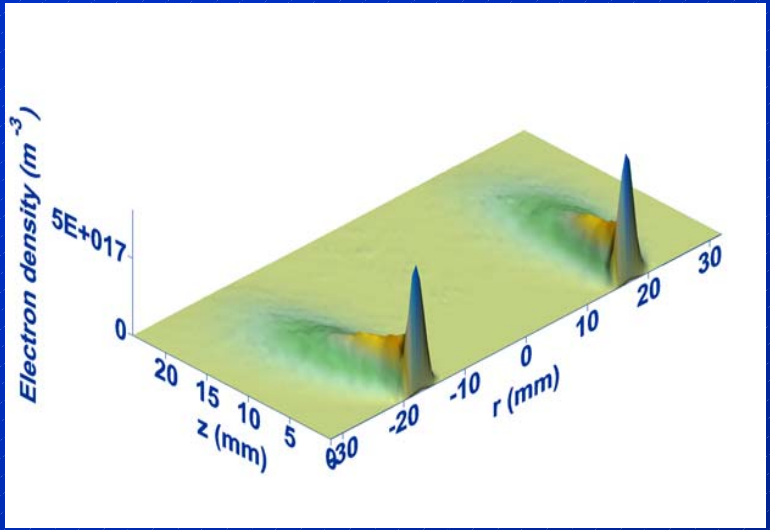


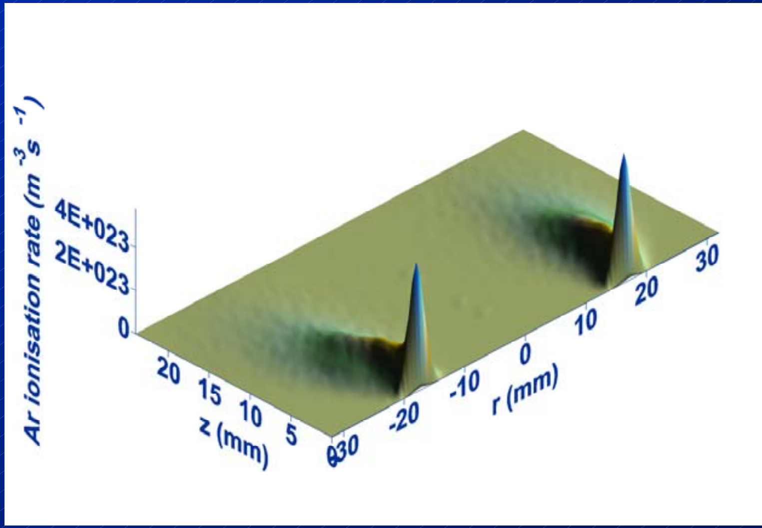
- Formation of a negative space charge region
- Strongly and weakly magnetized region
- Strong radial dependence
- Thin sheath ≈ 1 mm

Calculated Axial Electric Field, E_z



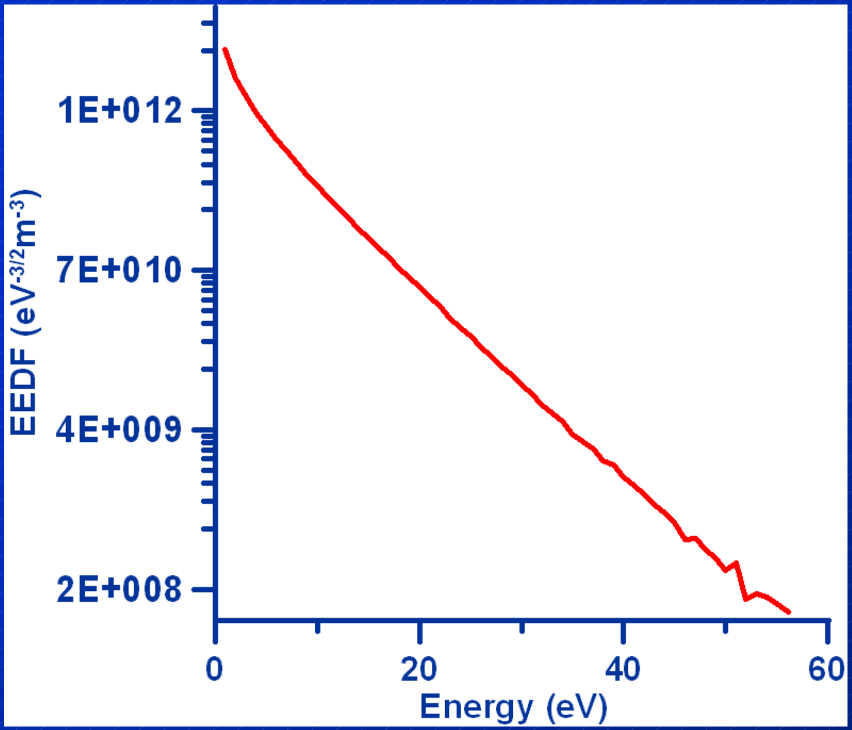
Calculated Electron Density and Ar Ionization Rate

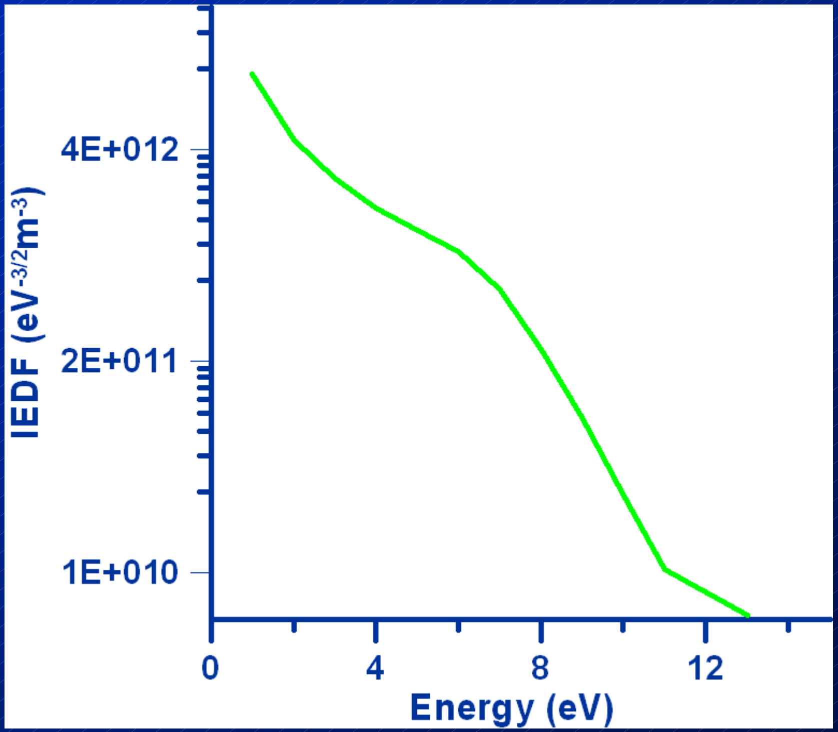




Very well confined plasma
Maximum – where B_r is maximal

Calculated Quasi-local EEDF and IEDF





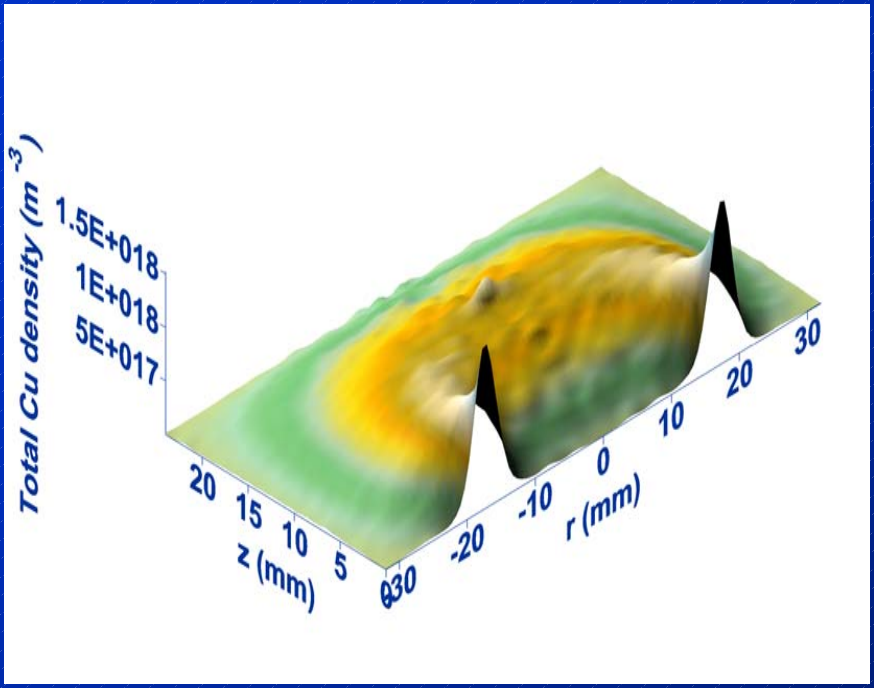
Essentially Maxwellian distribution

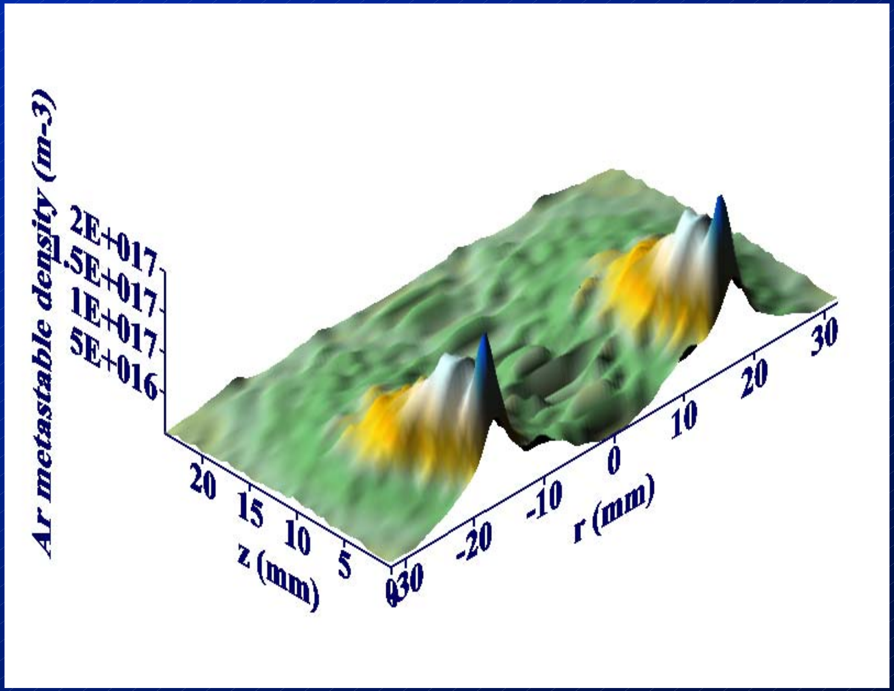
T_e = 14.2 eV

Severely non Maxwellian distribution

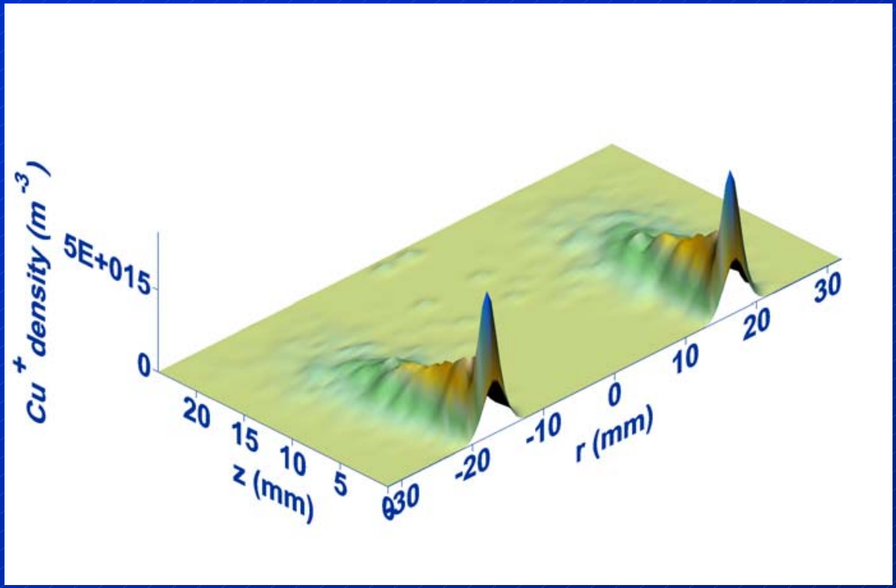
T_i not defined

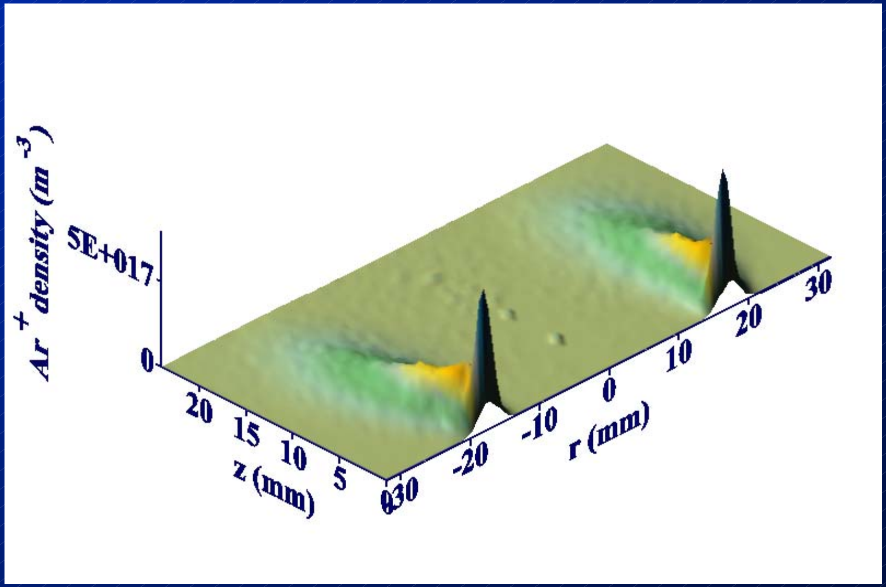
Calculated Cu and Ar* Density





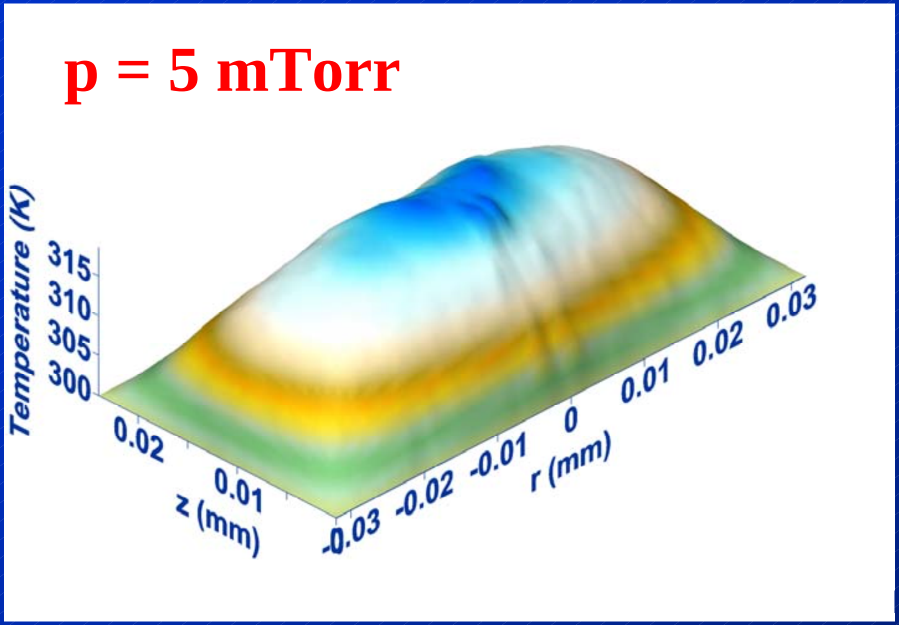
Calculated Cu⁺ Density and Ar⁺ Density

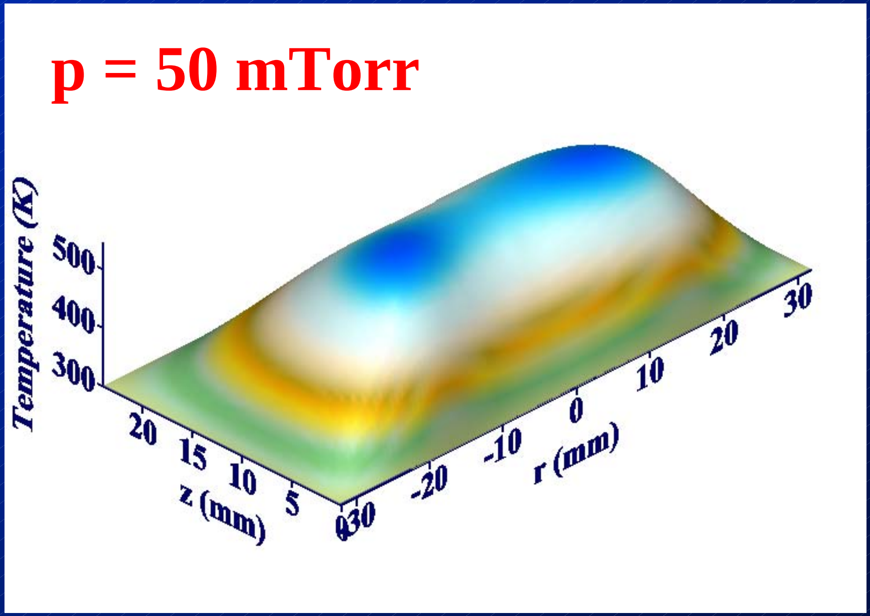




$$\frac{n_{Cu^+}}{n_{Ar^+}} \approx 10^{-2}$$

Ar Gas Temperature Distribution at 5 mTorr

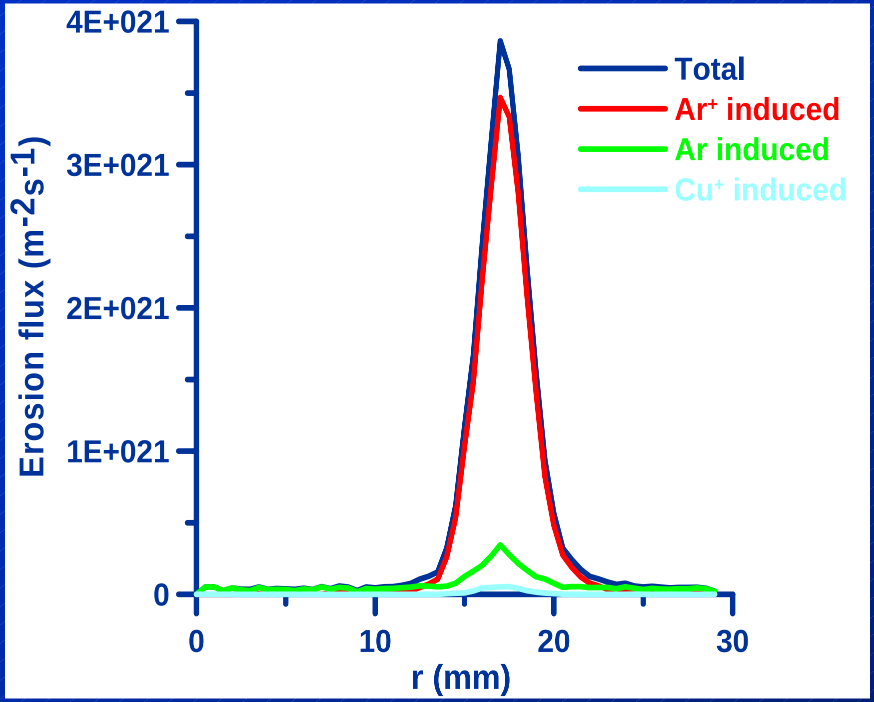


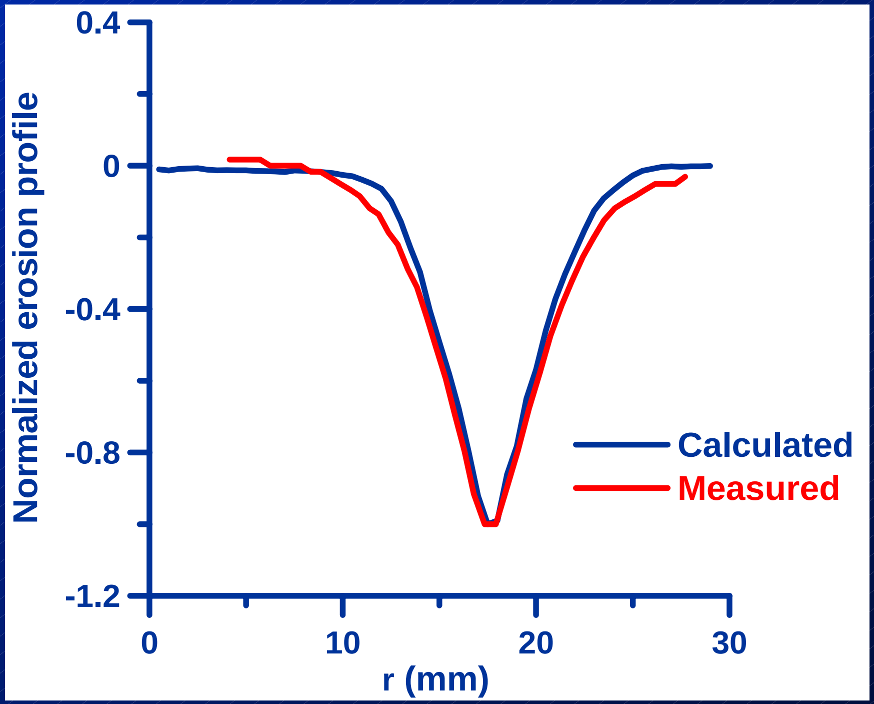


Main source: $Ar^f \rightarrow Ar^f$ elastic collisions

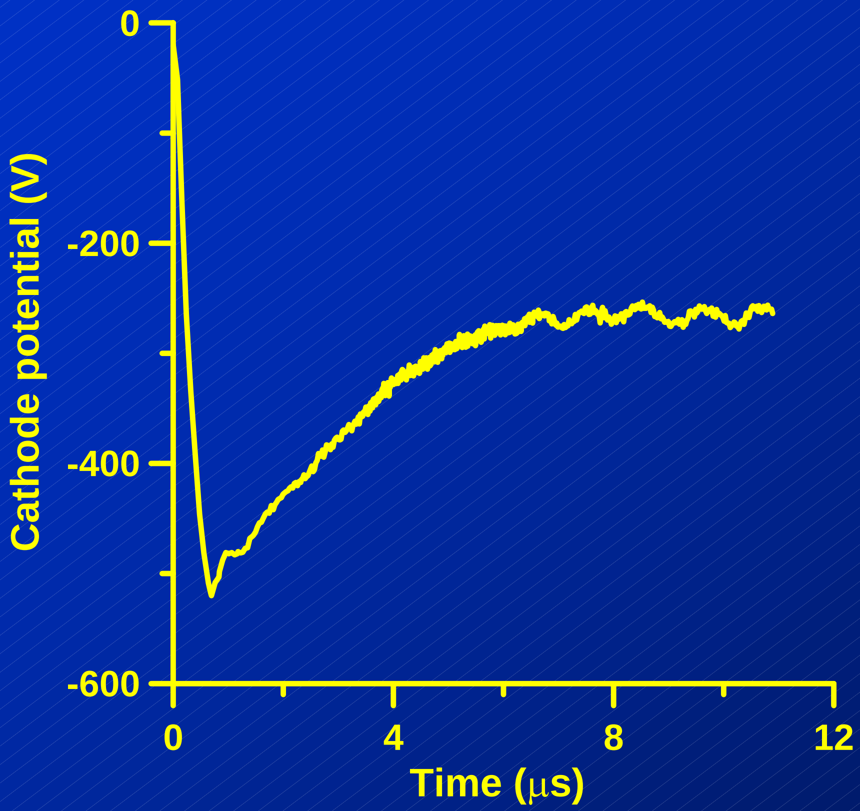
More significant contribution by Cu and Ar^+

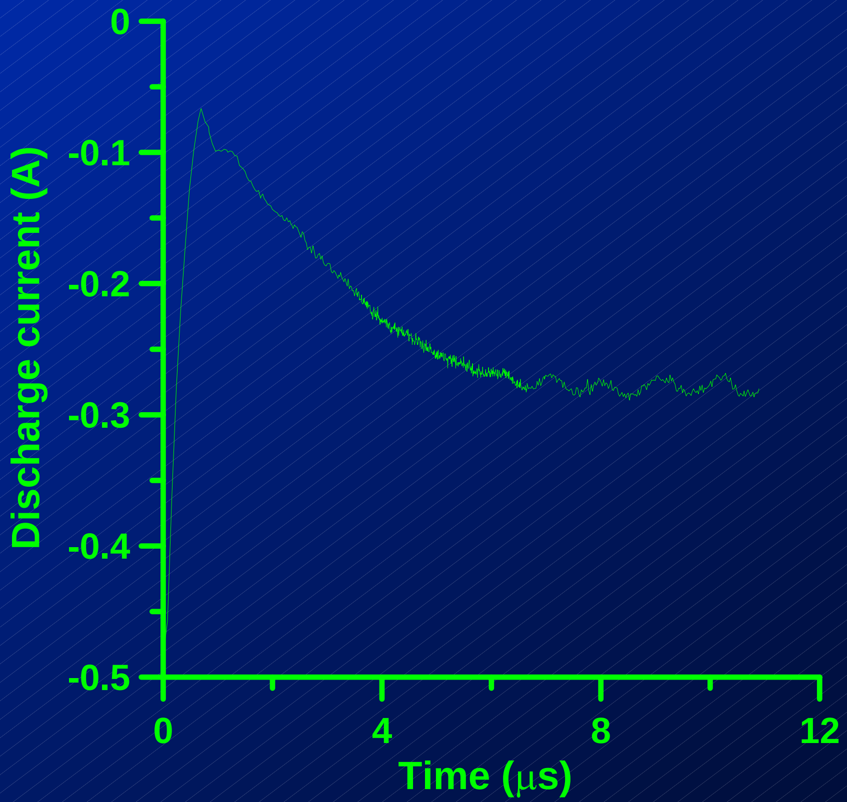
Relative Contribution of Ar^+, Ar and Cu^+ to the Sputtering of the Target

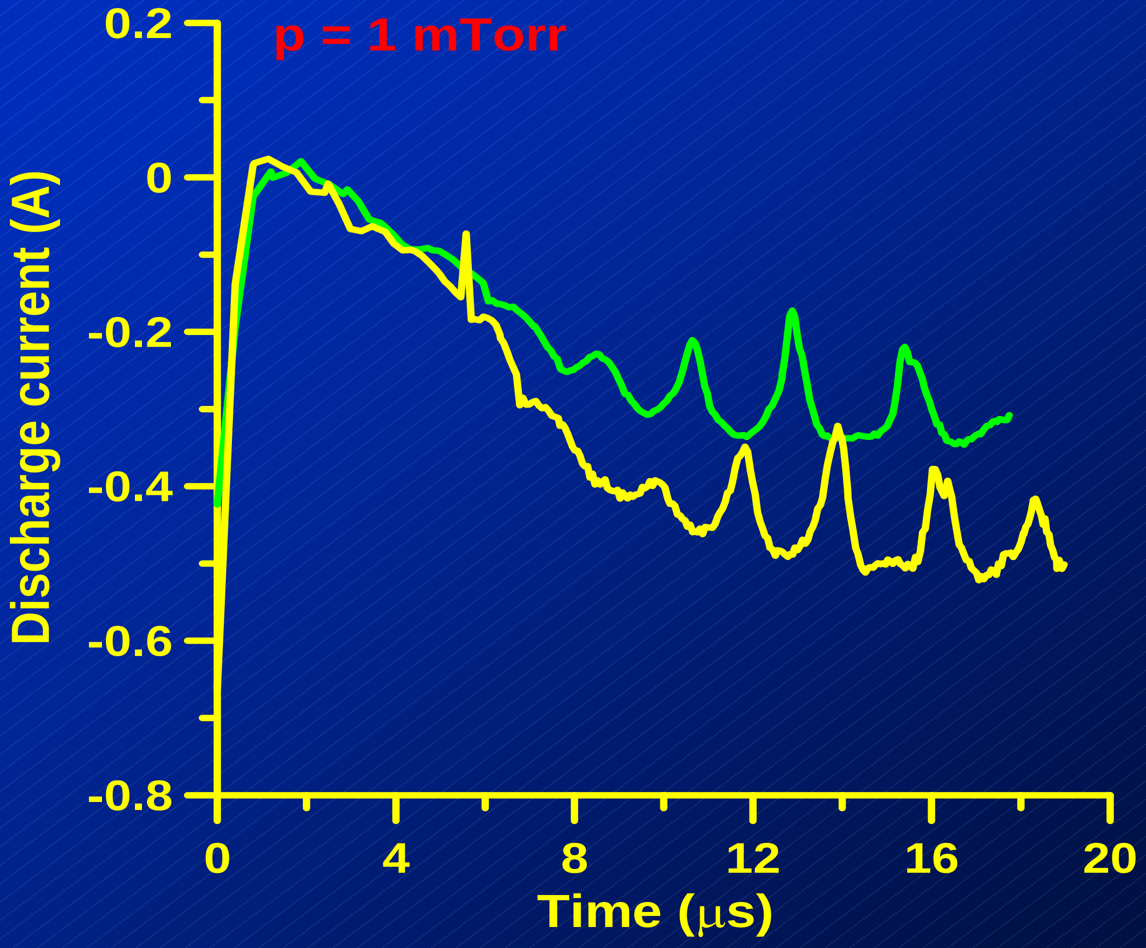




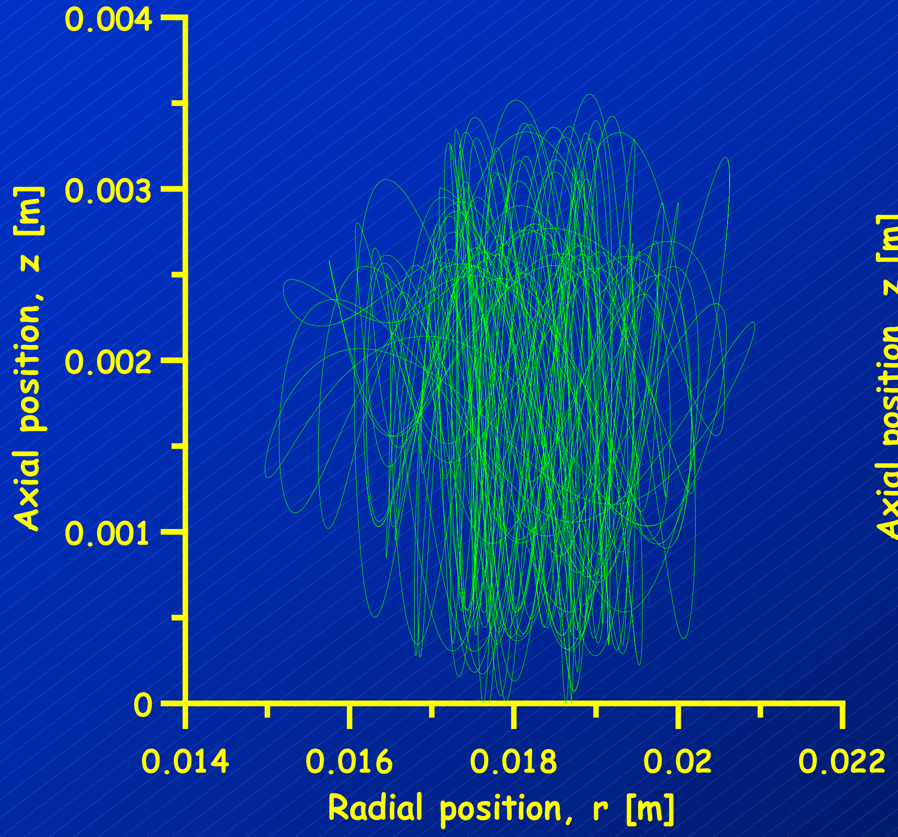
Convergence

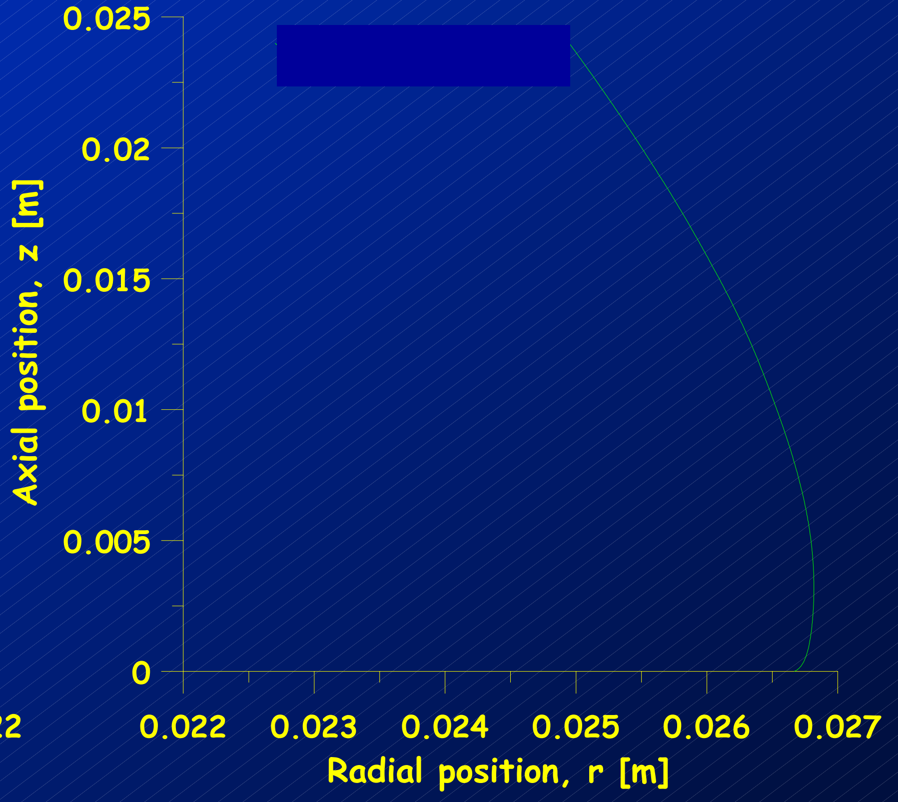




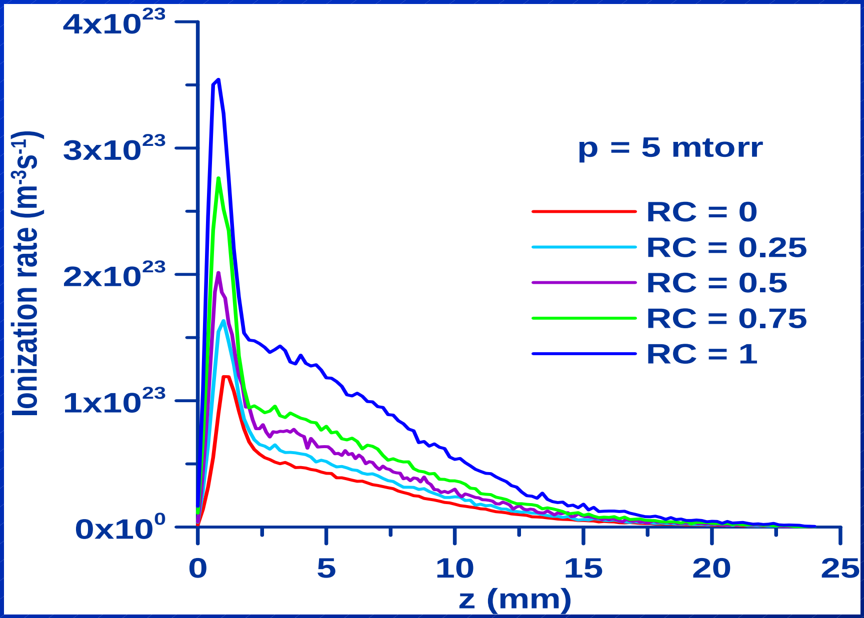

p = 1 mTorr
0.2
0
-0.2
-0.4
-0.6
-0.8
Discharge current (A)
0
4
8
12
16
20
Time (μs)

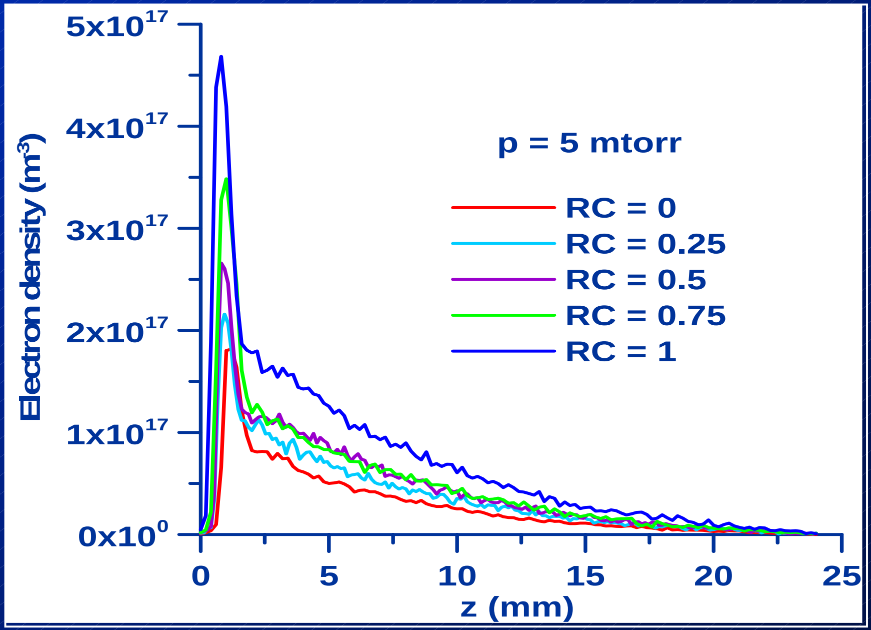
Electron Recapture at the Cathode





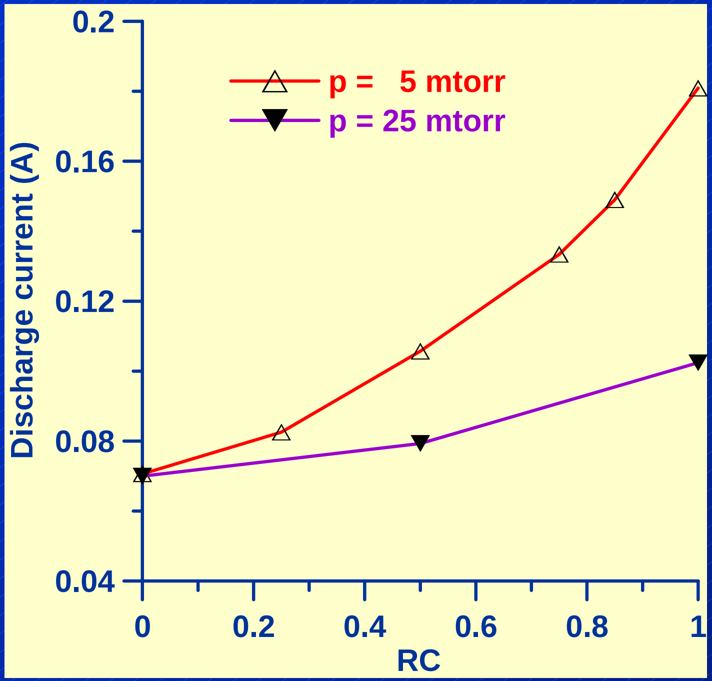
Electron Recapture at the Cathode: Influence upon the Discharge

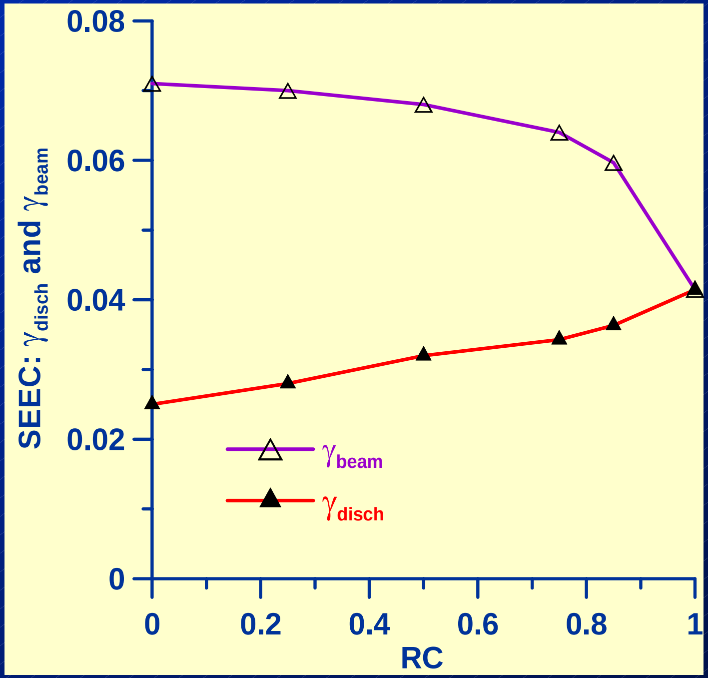




* $N_{ri=1} / N_{ri=0} = 2.8$

Electron Recapture at the Cathode: Influence upon the Discharge





- Changes conductivity

SEEC must be modified

Remedy:

fitting parameter (experimental data)

probabilistic treatment (Furman and Pivi, 2002)

Influence of the Magnetic field
p = 30 mTorr, r = 18.5 mm