Particle in Cell simulations of RF and DC break down

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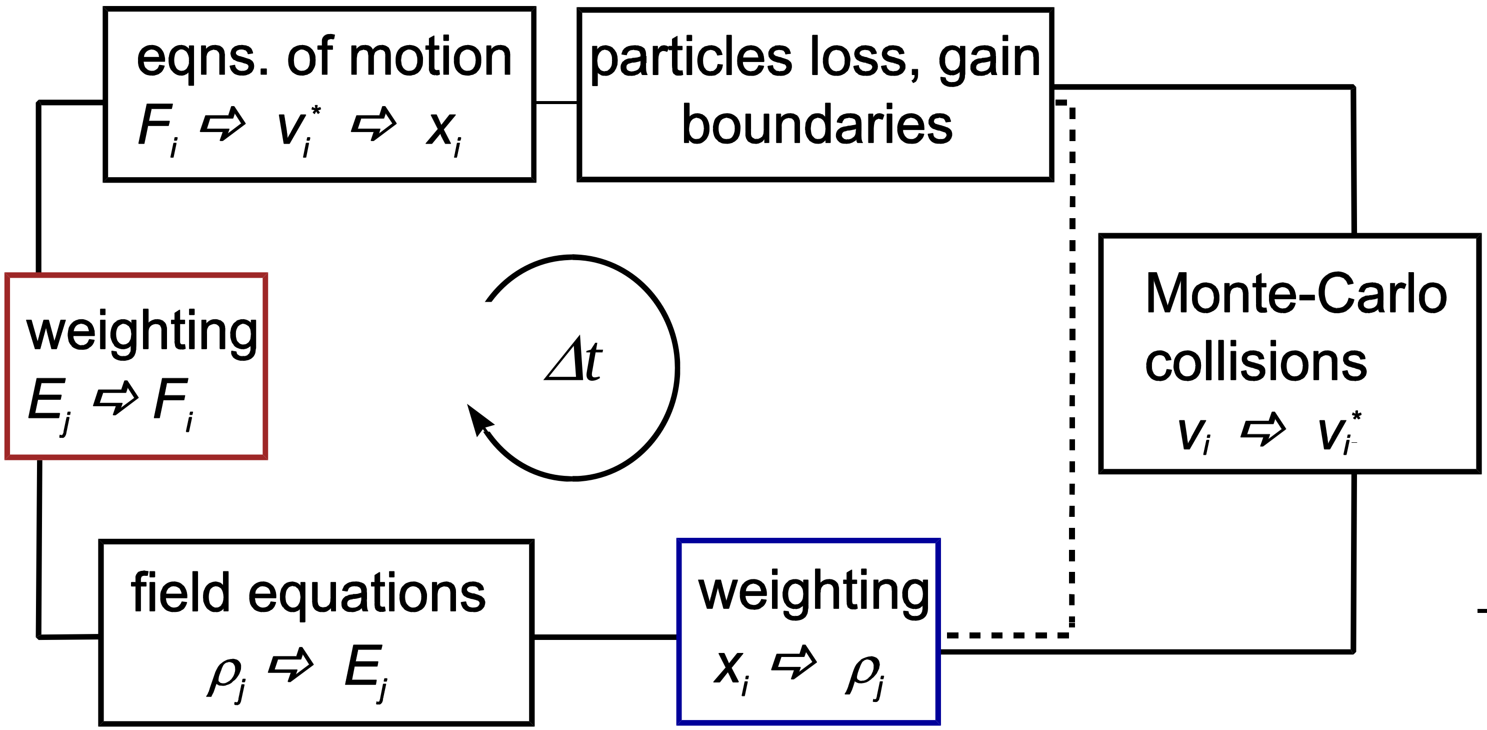
HGF-Junior research group “COMAS”:

Study of effects on materials in contact with plasma, either with fusion or low-temperature plasmas;

Development of computational multi-scale tools

Particle in Cell model

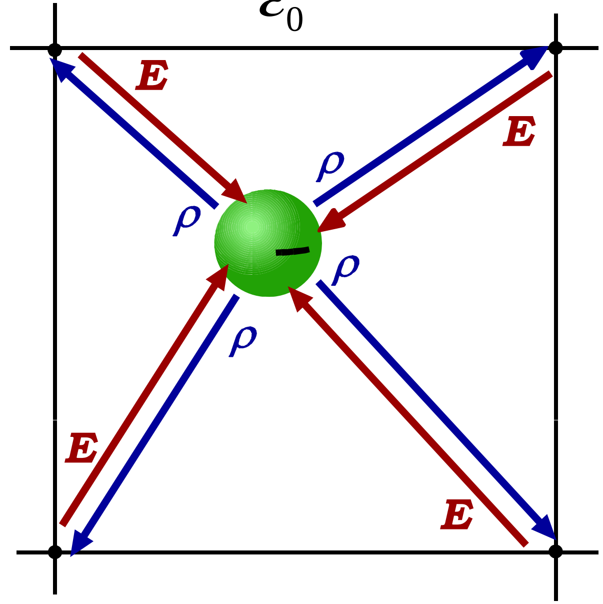


$$\frac{d\vec{x}}{dt} = \vec{v}$$

$$\frac{d\vec{v}}{dt} = \frac{q}{m}\left(\vec{E} + \vec{v} \times \vec{B}\right)$$

$$\vec{E} = -\nabla \varphi$$

$$\Delta\varphi = -\frac{1}{\varepsilon_0}\rho(x)$$



$$\rho = \sum_i \frac{q_i}{\Delta x \Delta y} S(x - x_i)$$

$$S(x) = \begin{cases} \left(1 - {|x|}/{\Delta x}\right)\left(1 - {|y|}/{\Delta y}\right) & |x| \le \Delta x \quad and \quad |y| \le \Delta y \\ 0 & \end{cases}$$

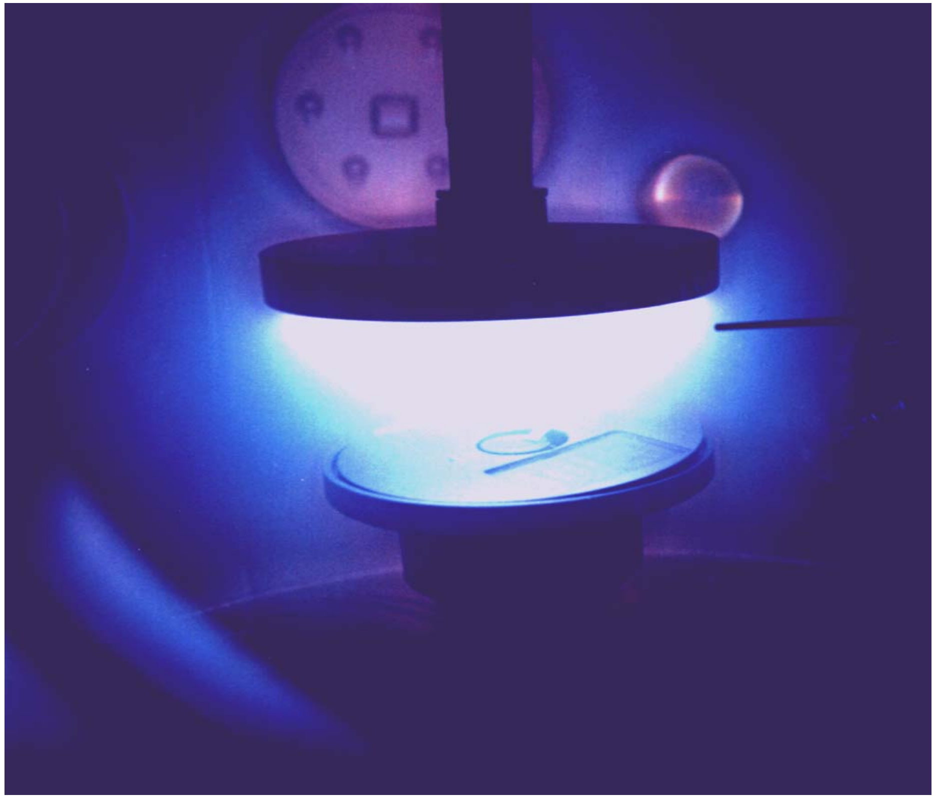
PIC simulation: RF capacitive discharge

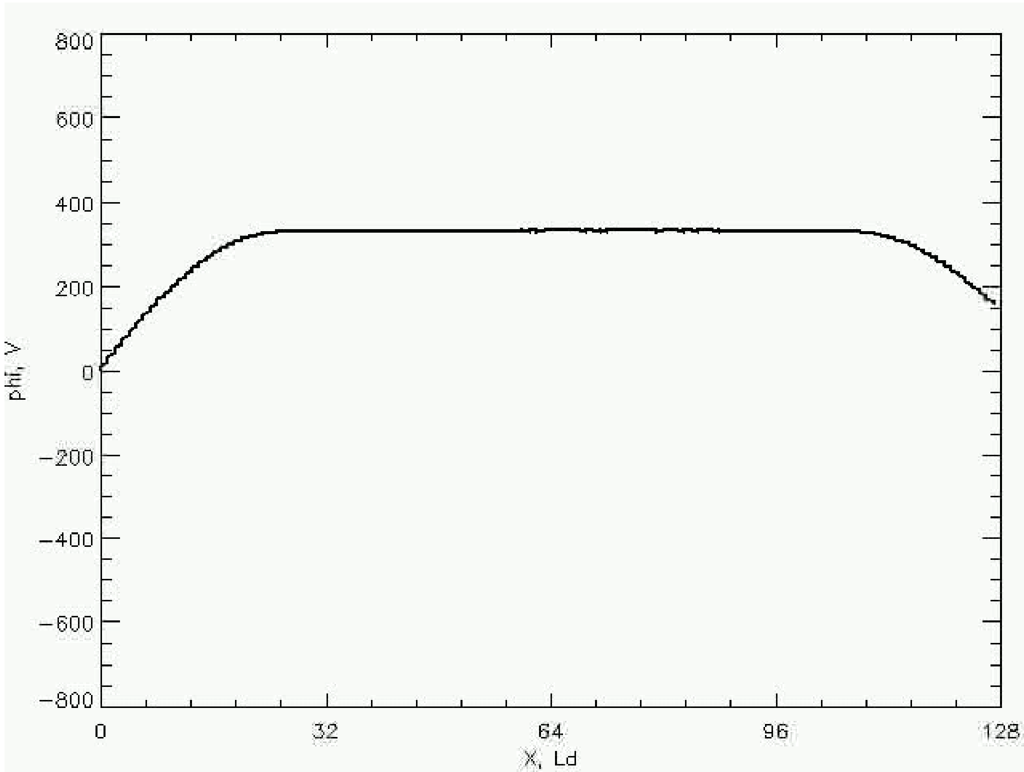
Parallel plate RF discharge

f_{RF} = 13.56 MHz , RF peak-to-peak voltage ~ 200 -1600 V

Gas : Oxygen, pressure p = 1 - 100Pa, electron density $n_e \sim 10^9 - 10^{10}$ cm^{-3}

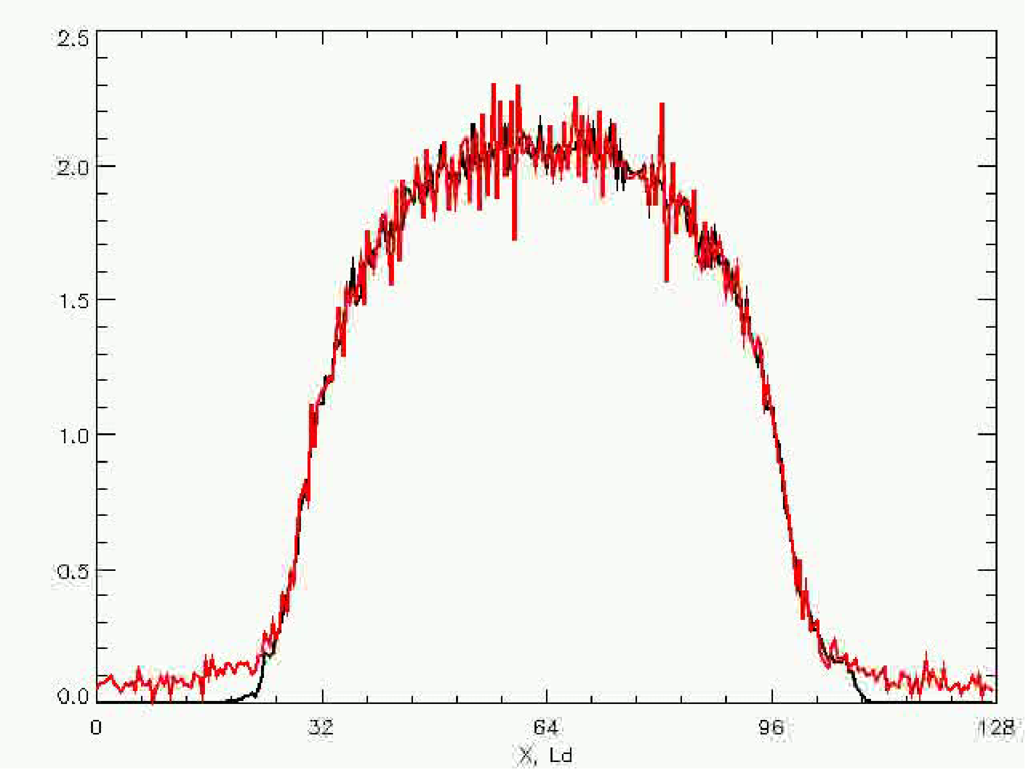
potential



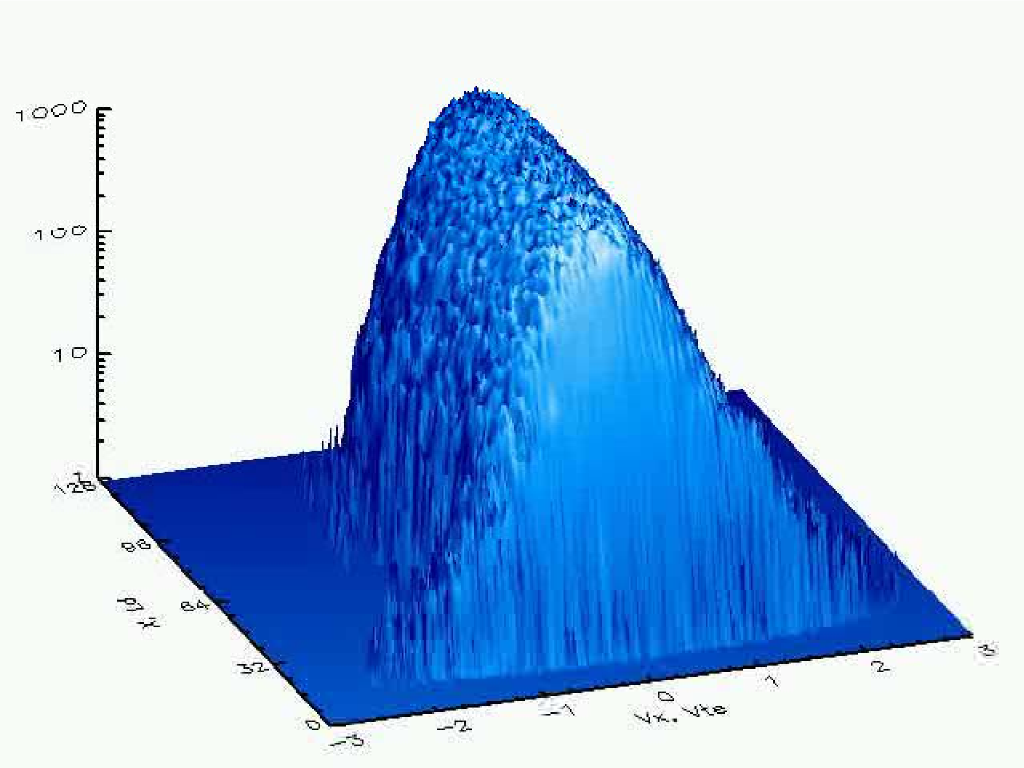


PIC simulation: RF capacitive discharge

Electron and O_2^+ density, 10^9 cm^{-3}



electron parallel velocity distribution
10 Pa, 250 V



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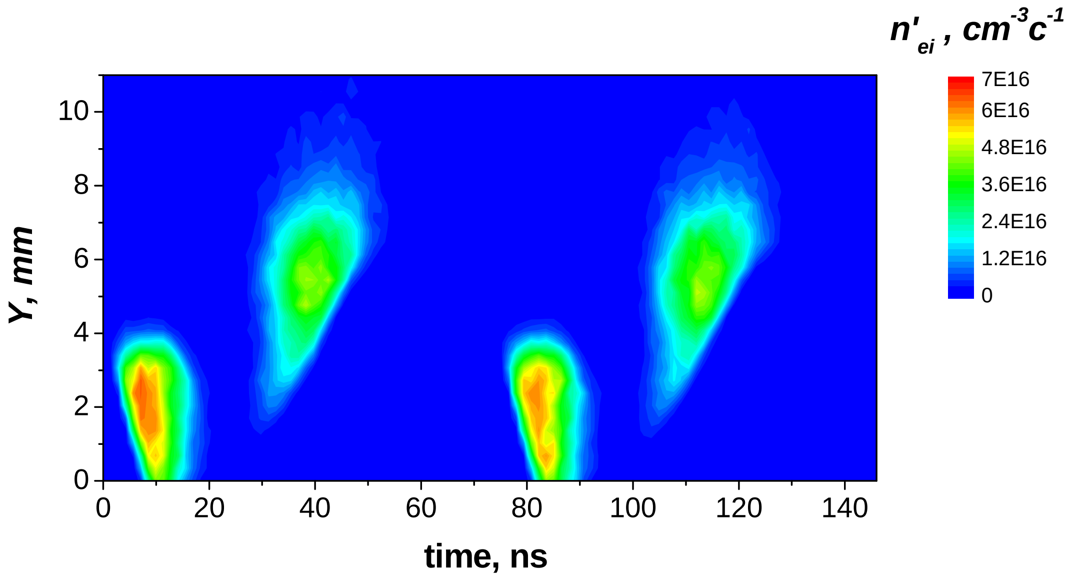
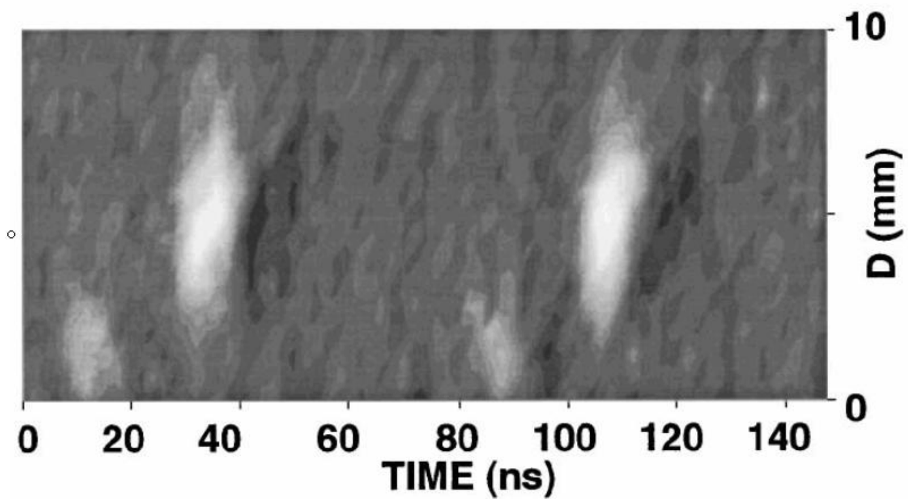
PIC simulation: RF capacitive discharge

electron-impact ionization rate
simulation



653.3 nm excitation rate
experiment



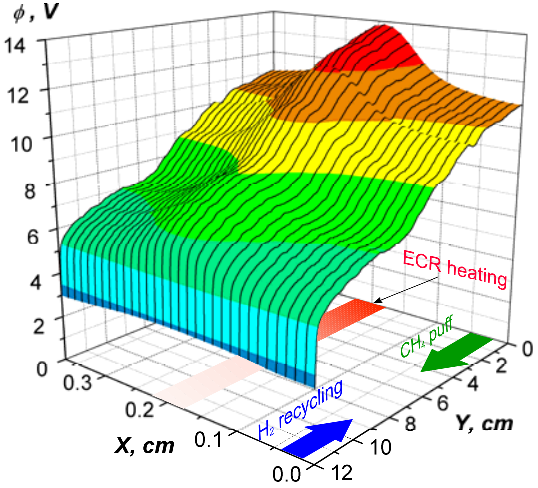
C.M.O. Mahony et al.,
Appl. Phys. Lett. ***71*** *(1997) 608.*

double peak structure due to sheath reversal

Particle-in-Cell code applications

ECR plasma

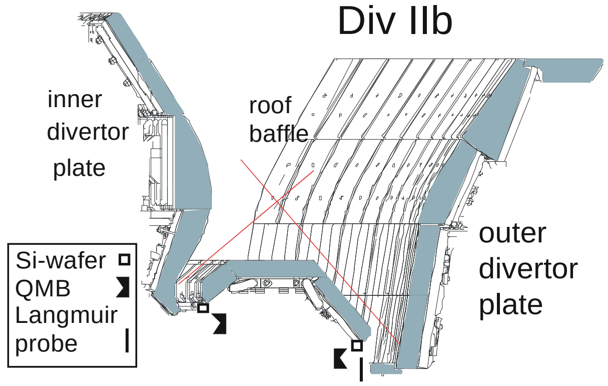
$n_e \sim 10^{10}\ cm^{-3}$
$n_n \sim 10^{14}\ cm^{-3}$
$T_e \sim 2\ eV$



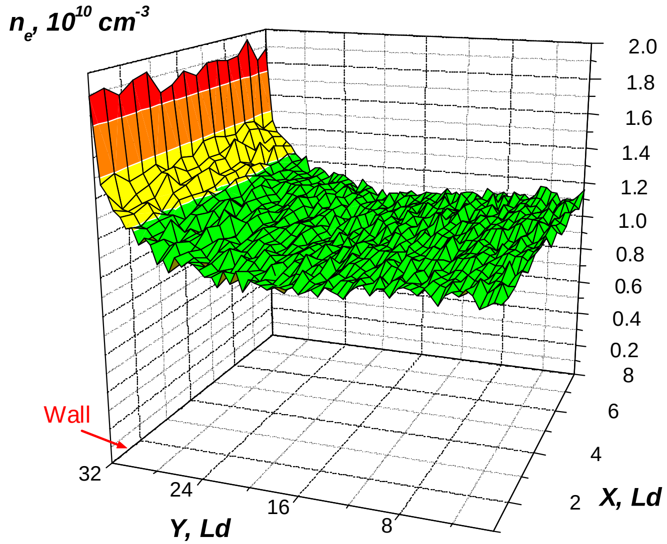
Parasitic plasma under AUG divertor

Plasma detected below roof baffle of Div IIb

Typical parameters:
$4 \cdot 10^8 < ne < 7 \cdot 10^{11}\ cm^{-3}$
$5 < Te < 15\ eV$
Scaling: $ne \sim Radiation^{2.7} \cdot Particles\_flux^{0.7}$

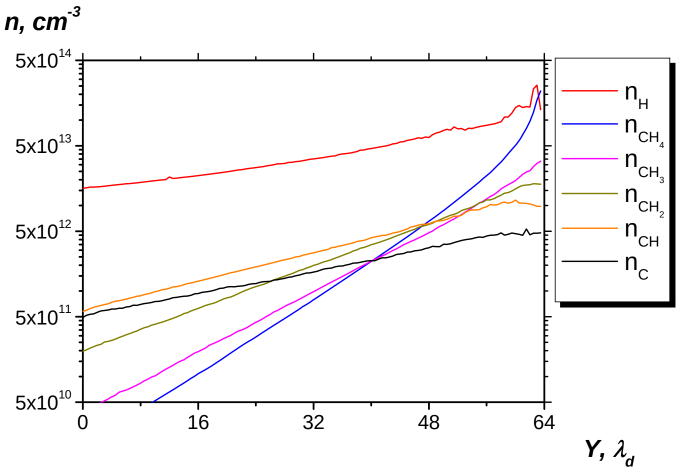


Plasma originated by photoionisation or photoeffect !



Recycling in SOL

$n_e \sim 10^{13}\ cm^{-3}$
$n_n \sim 10^{14}\ cm^{-3}$
$T_e \sim 10\ eV$



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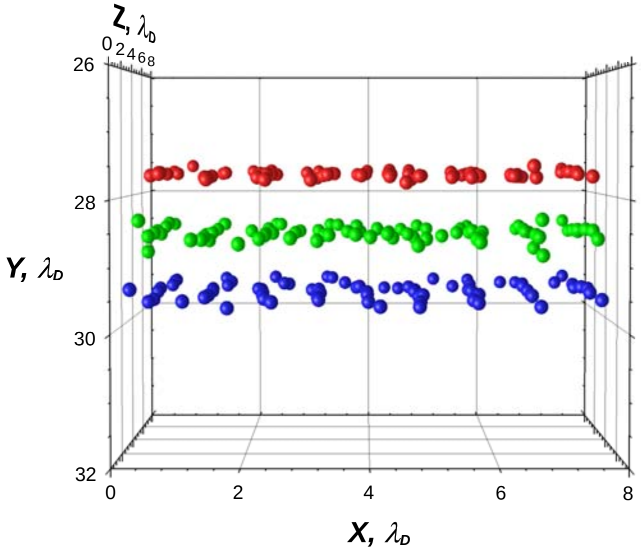
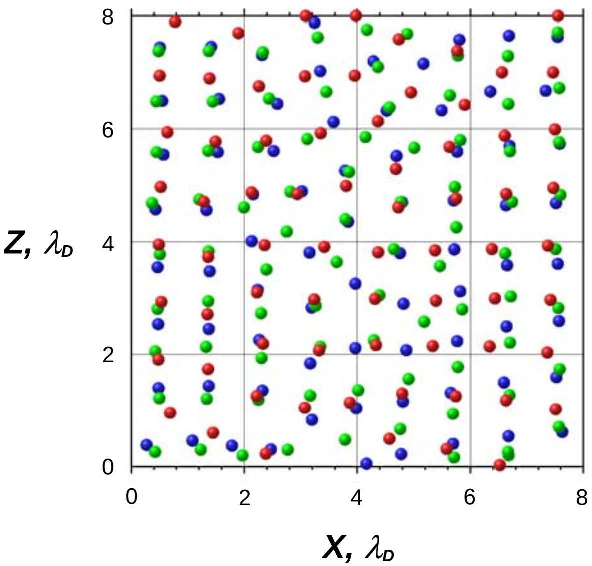
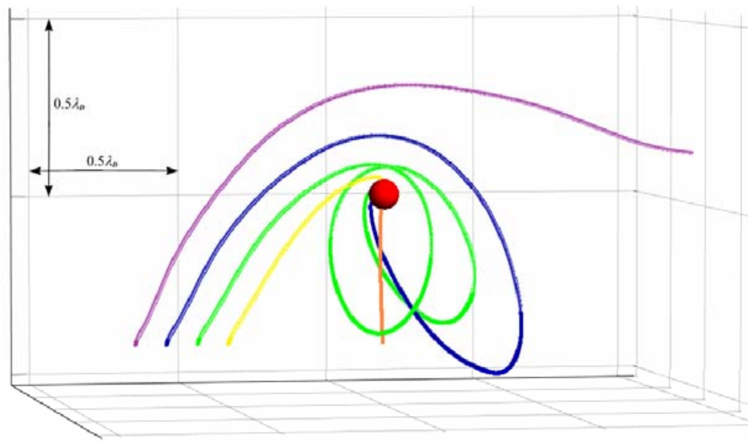
Particle-in-Cell code applications

Dusty plasmas and plasma crystals

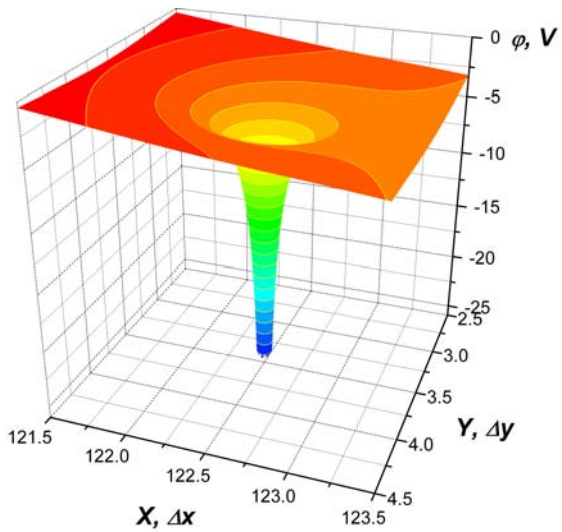




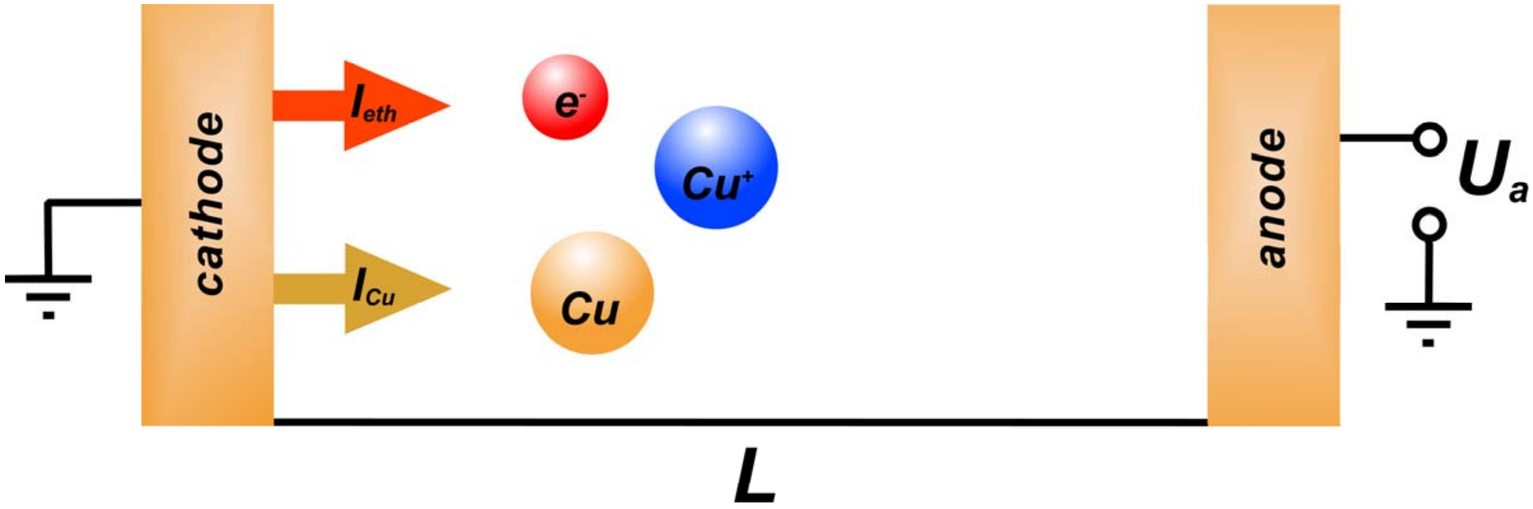
Ion trajectories close to the dust grain



Potential close the dust grain



PIC modeling of arcing: DC discharge



L **= 20 μm**
U_a **= +10 kV**

Species included: e^-, Cu^+, Cu

- electrodes material is Copper.
- the constant electron thermo-emission current $\boldsymbol{I_{eth} = 2.35 \cdot 10^6}$ **A/cm²** from the cathode is assumed.
- the constant flux of evaporated copper atoms from the cathode $\boldsymbol{I_{Cu} = 0.1 I_{eth}/e}$ is assumed

Simplistic surface interaction model:

- each Cu^+ ion hitting electrode surface sputters the Cu atom with probability 100%
- each electron hitting the electrode surface sputters the Cu atom with probability 1%.
- each Cu atom hitting surface is reflected back

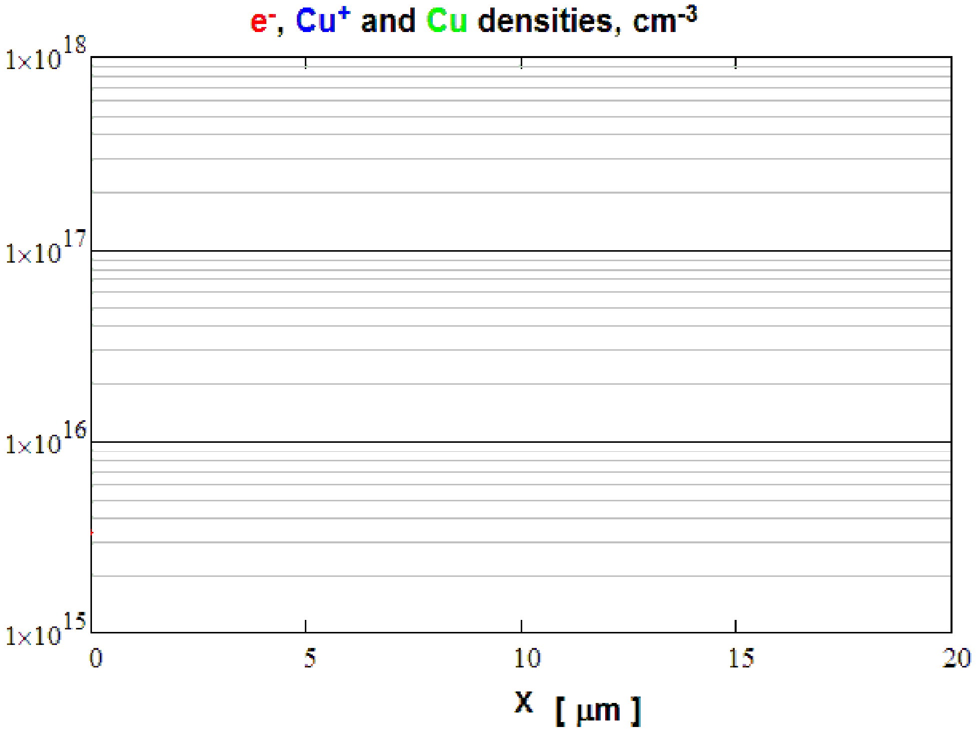
Collisions:

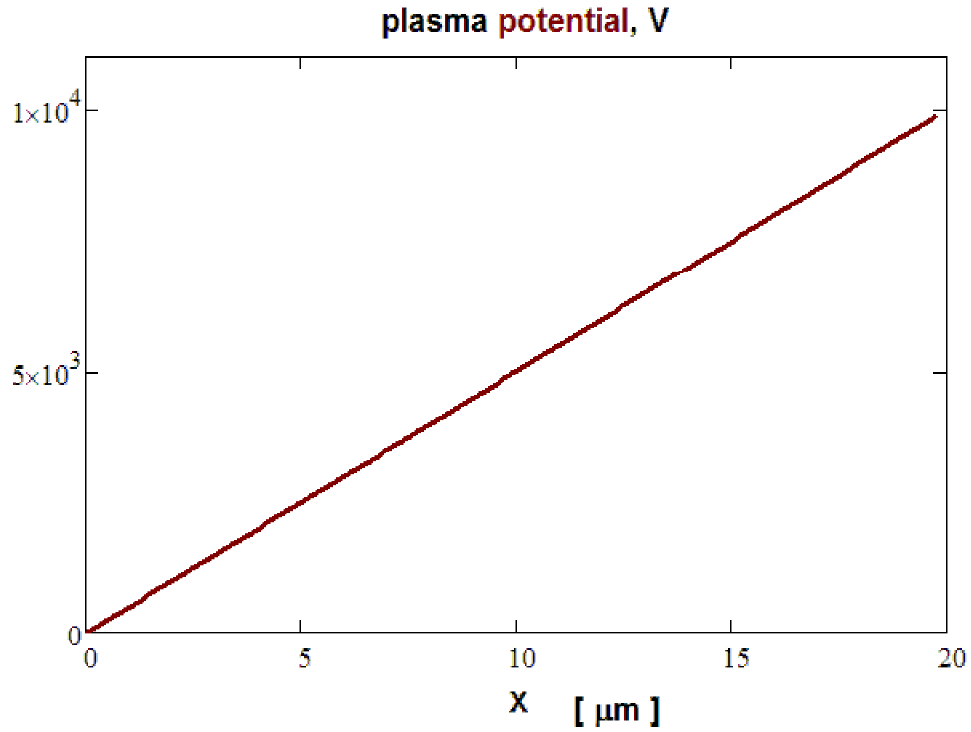
Coulomb collisions for the (e^-,e^-), (Cu^+,Cu^+) and (e^-, Cu^+)

e^- + Cu	=> e^- + Cu	electron - neutral elastic collision
e^- + Cu	=> $2e^-$ + Cu^+	electron impact ionization
Cu^+ + Cu	=> Cu^+ + Cu	charge exchange and momentum transfer
Cu + Cu	=> Cu + Cu	elastic collisions

PIC modeling of arcing: DC discharge

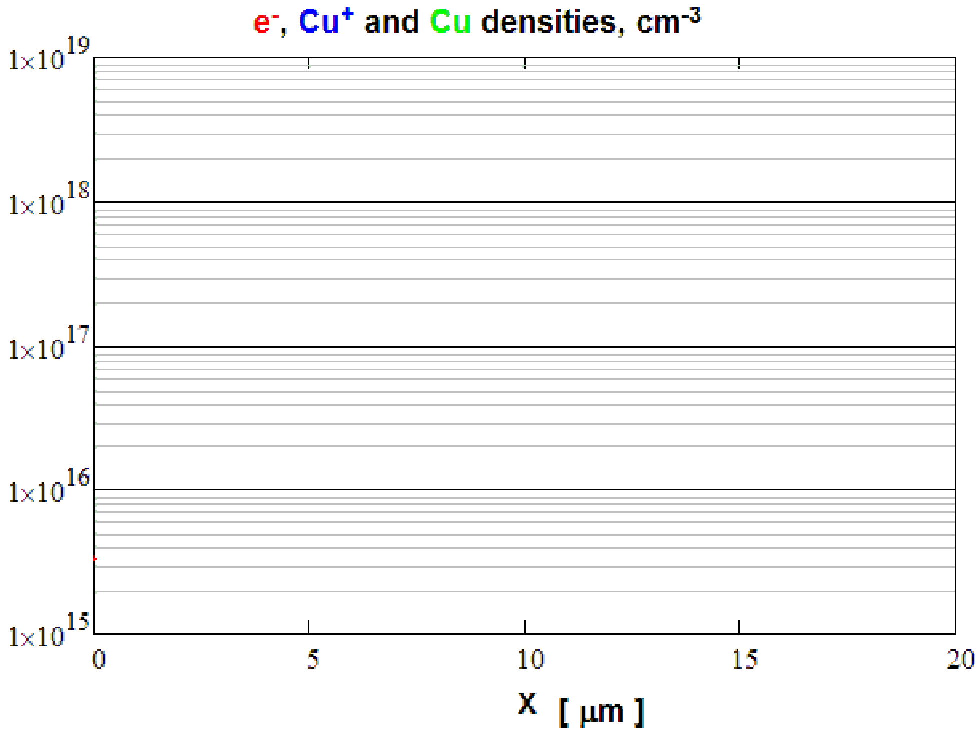
Start-up phase of the discharge (the first 0.7 ns)

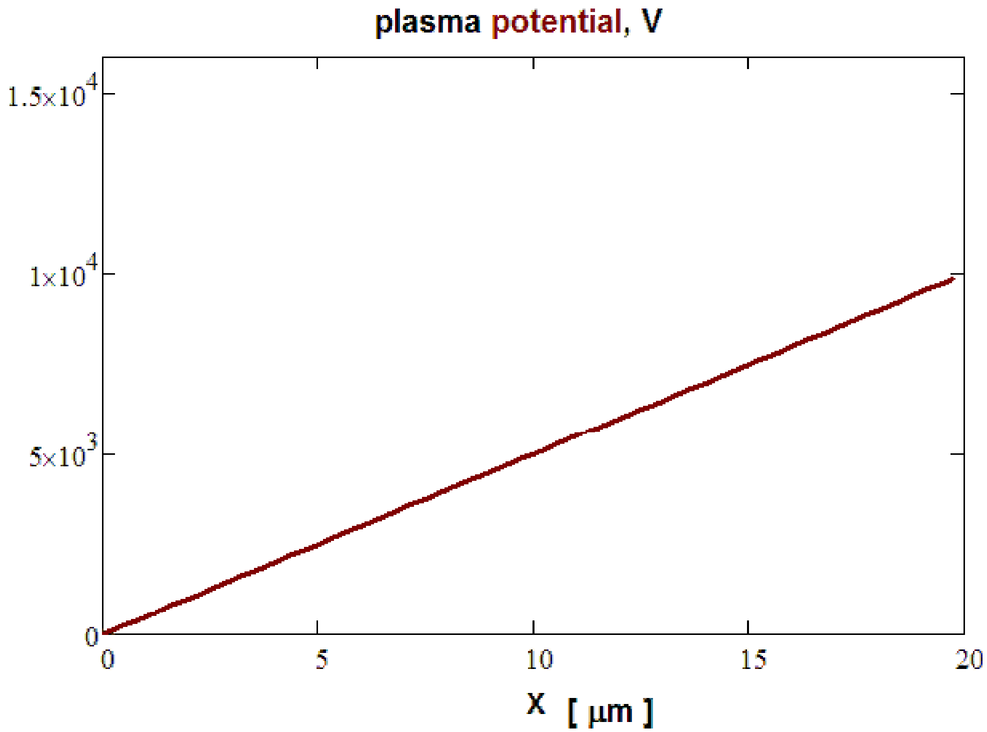




PIC modeling of arcing: DC discharge

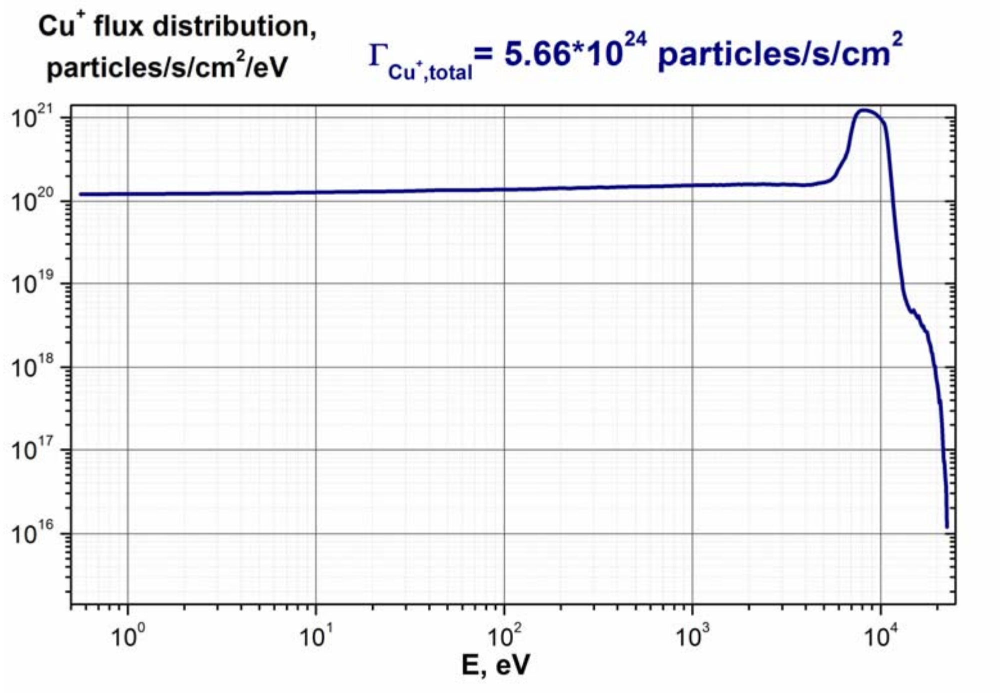
Simulated time 18 ns





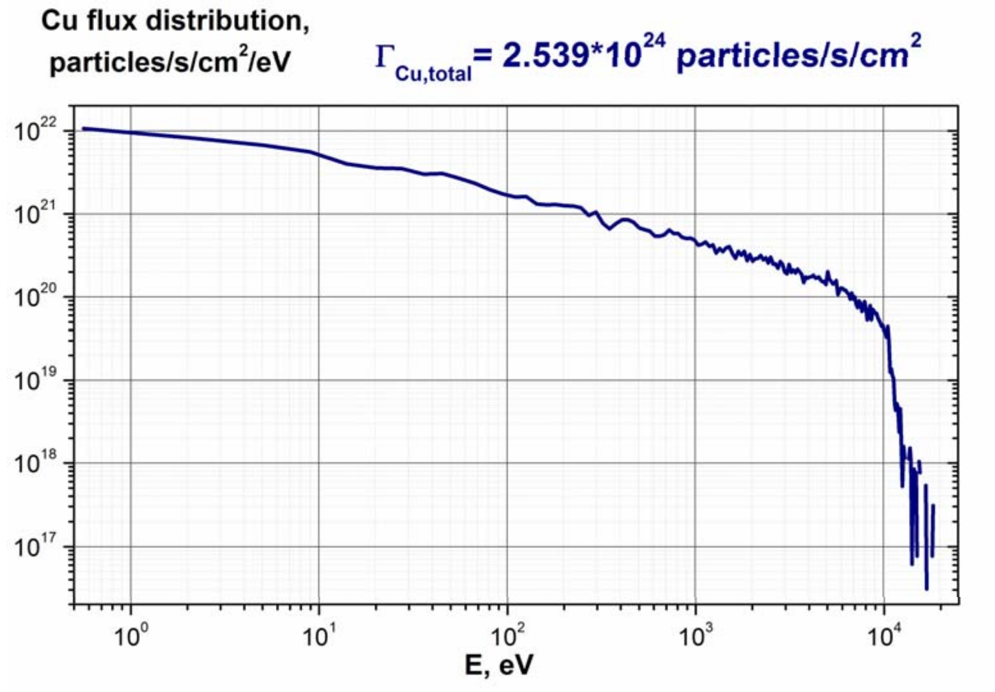
PIC modeling of arcing: DC discharge

Cu^+ flux energy composition at the cathode



Maximum energy corresponds to sheath potential drop
Lower enrery part is populated by collisions with neutrals

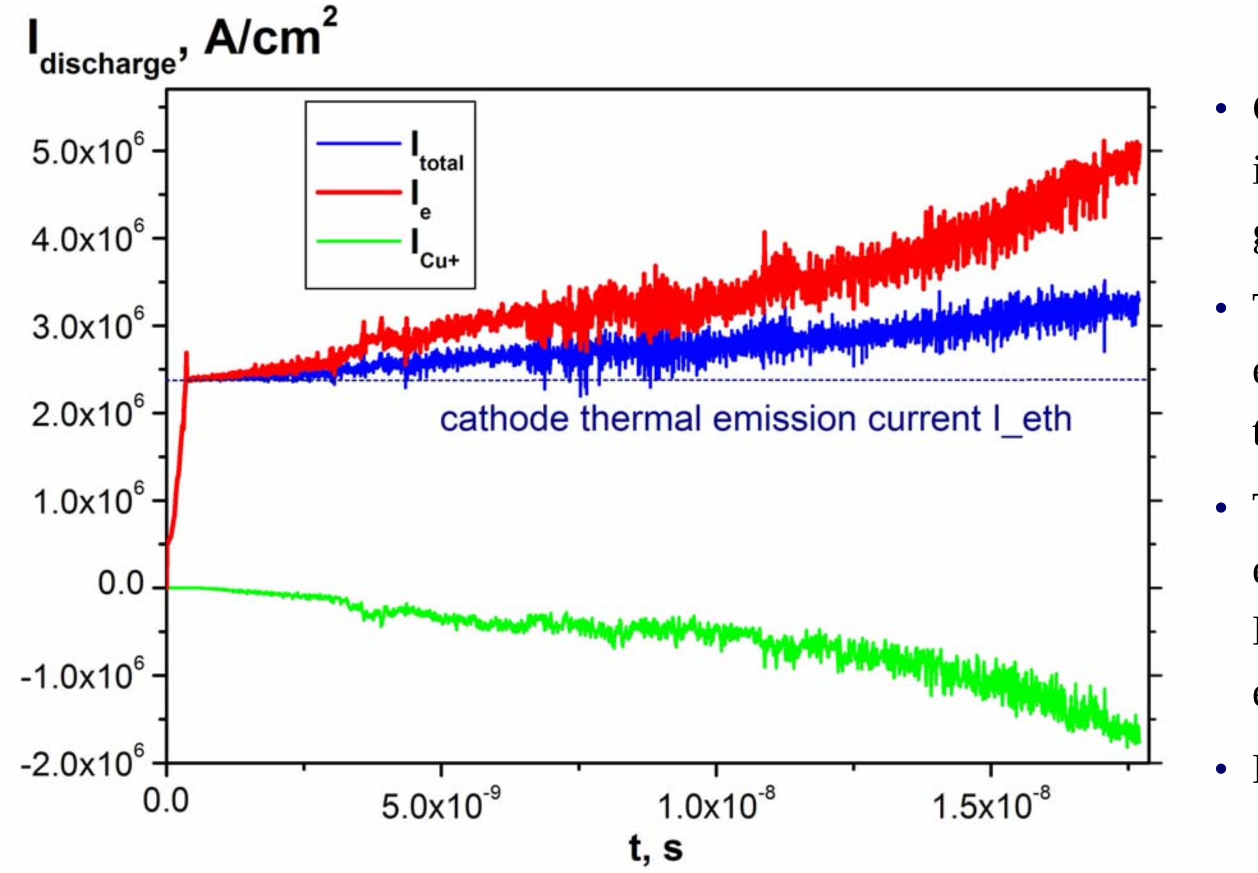
Cu flux energy composition at the cathode



High energy neutrals due to charge exchange

PIC modeling of arcing: DC discharge

Discharge current to anode



Main results:

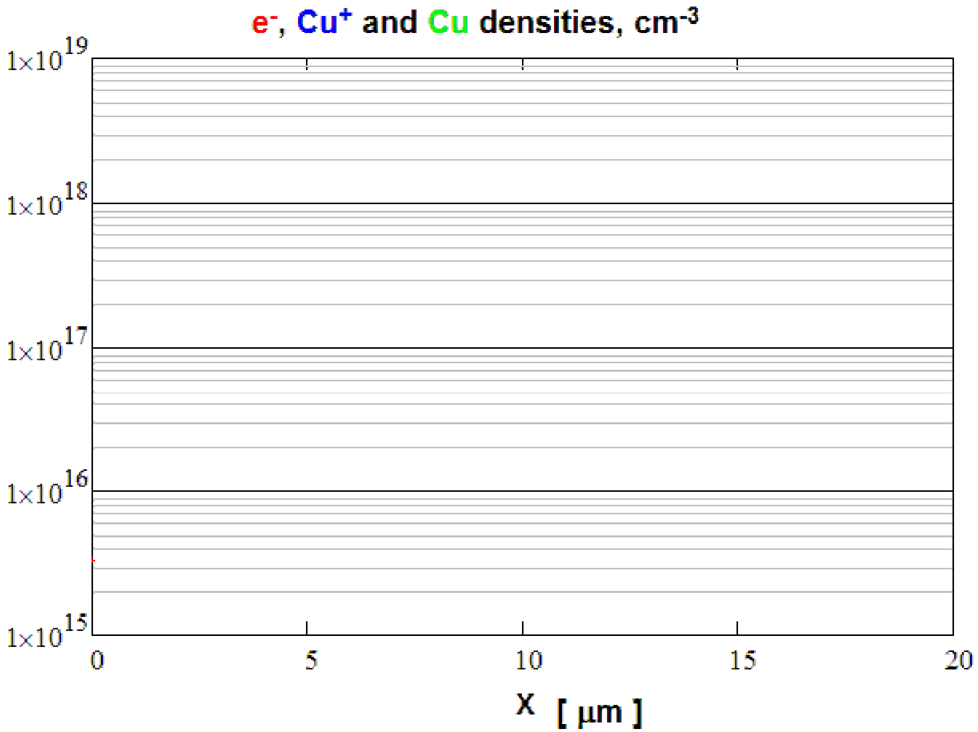
- **Cu** atoms evaporated from cathode are ionized by the electrons accelerated in the gap, creating $\mathbf{e^-}$, $\mathbf{Cu^+}$ plasma
- The flux of the plasma particles to the electrodes enhances the sputtering, increasing the concentration of the **Cu** atoms in the gap
- The plasma space charge start to influence the external electric field in the gap when the Debye length becomes smaller then the electrode spacing.
- Electric field is concentrated in sheath $\sim 8\lambda_{De}$

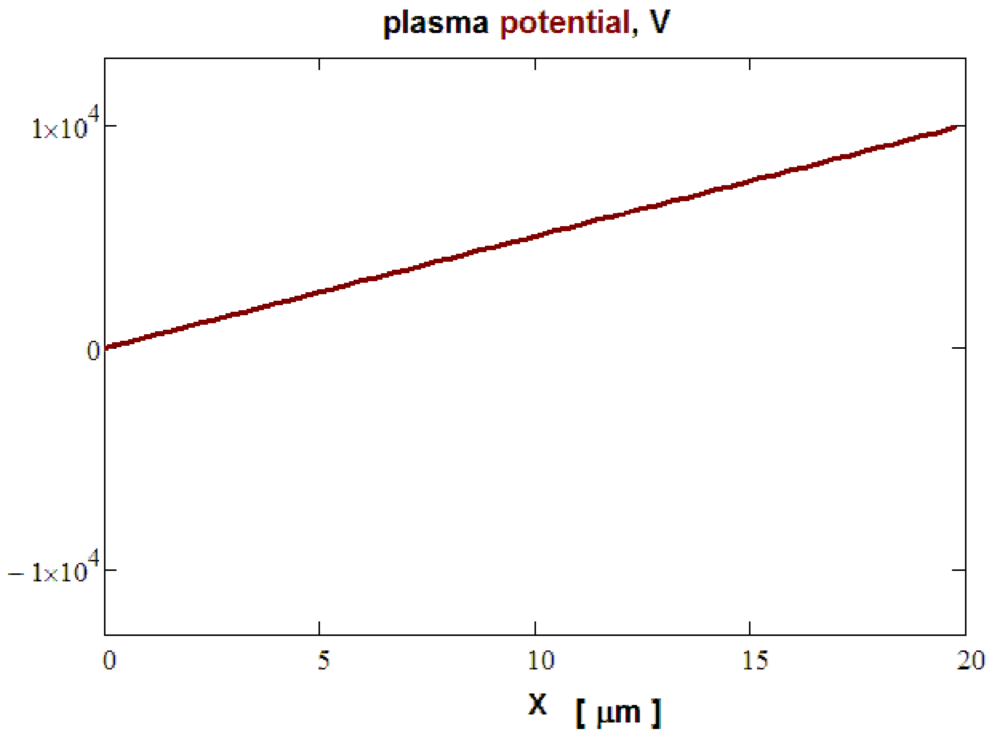
$$\lambda_{De} = \sqrt{\frac{\varepsilon_0 k T_e}{n_e e^2}}$$

PIC modeling of arcing: RF discharge

Same geometry and the model as for DC case,
only now right electrode is powered with RF voltage U_{RF} **= 10 kV,** f_{RF}**= 11.75 GHz**

Simulated time ~18 ns

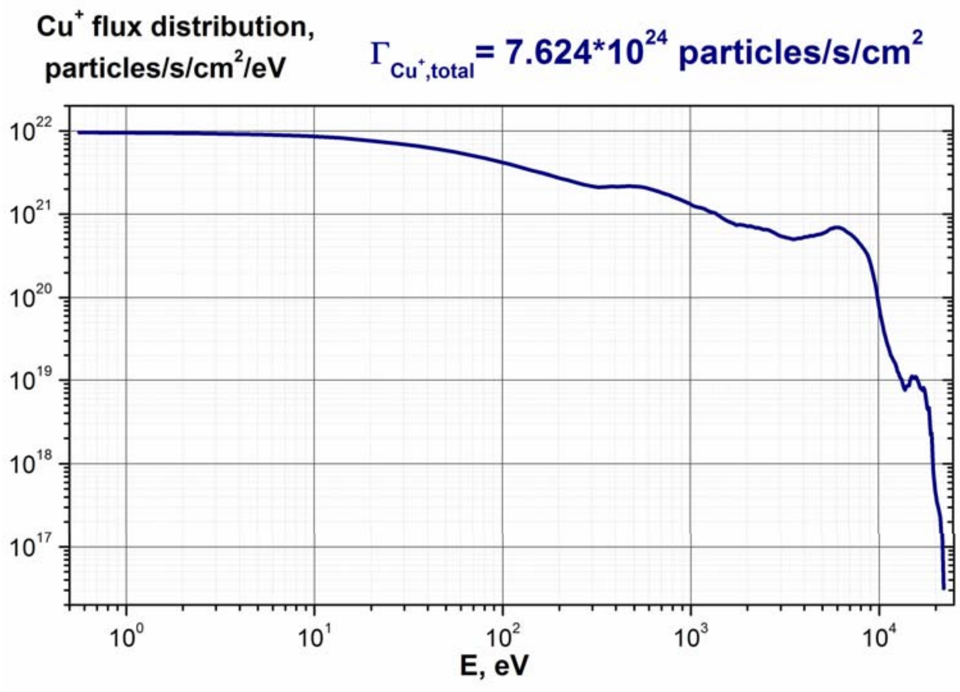




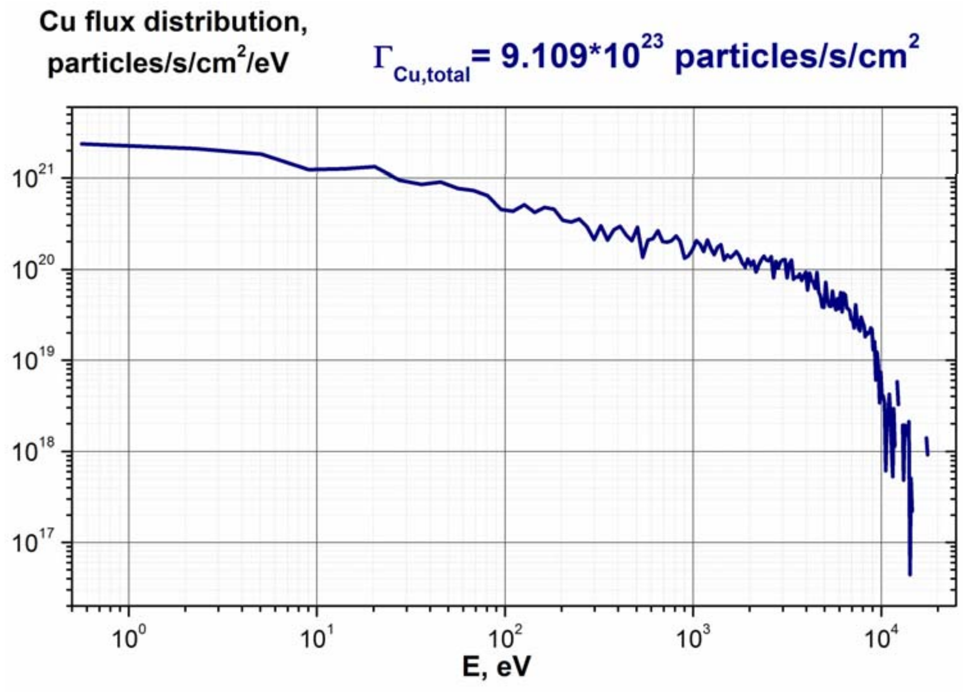
*Here frames are taken at 13/12*T_{RF} *, so one can see RF dynamics*

PIC modeling of arcing: RF discharge

Cu^+ flux energy composition at the powered electrode

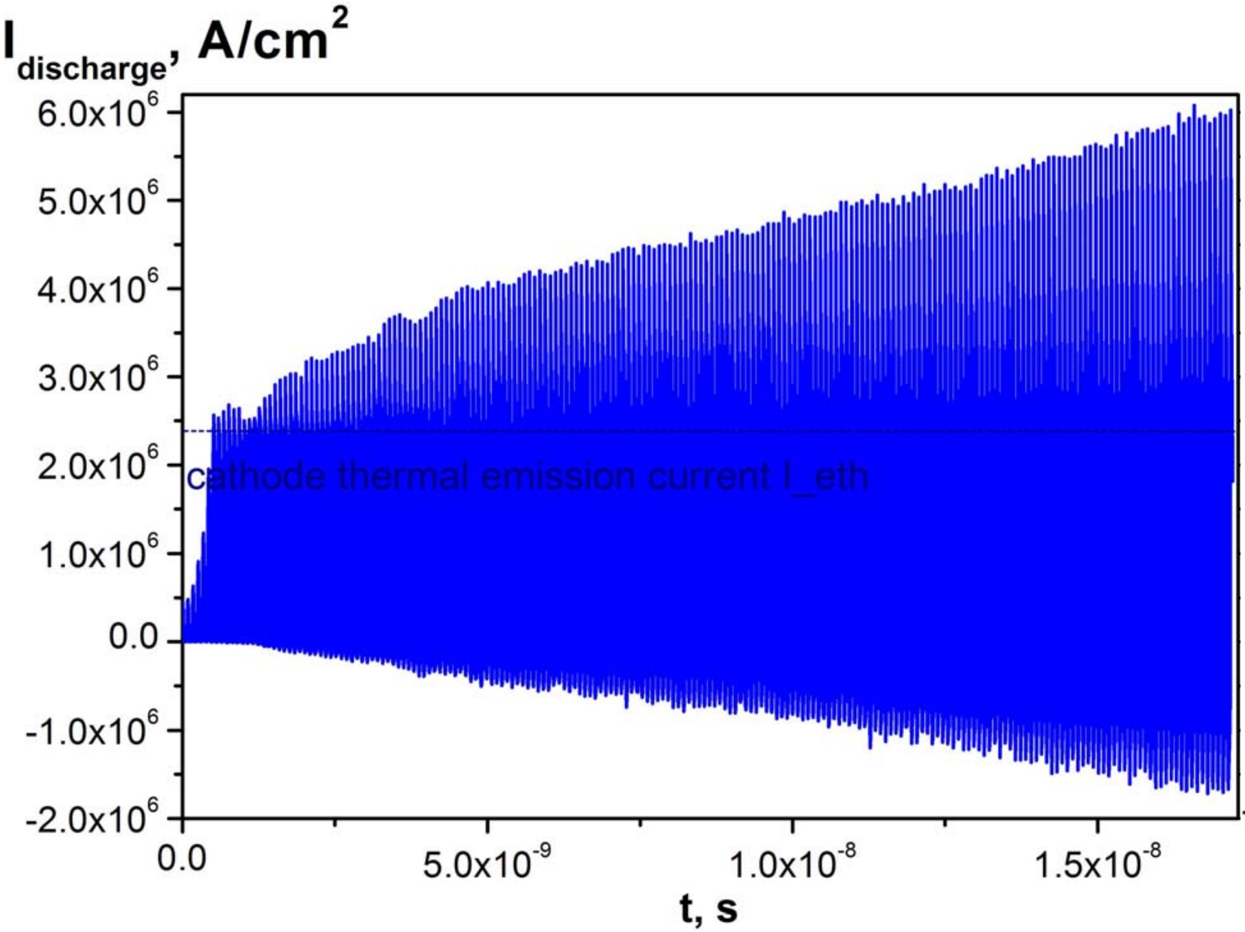


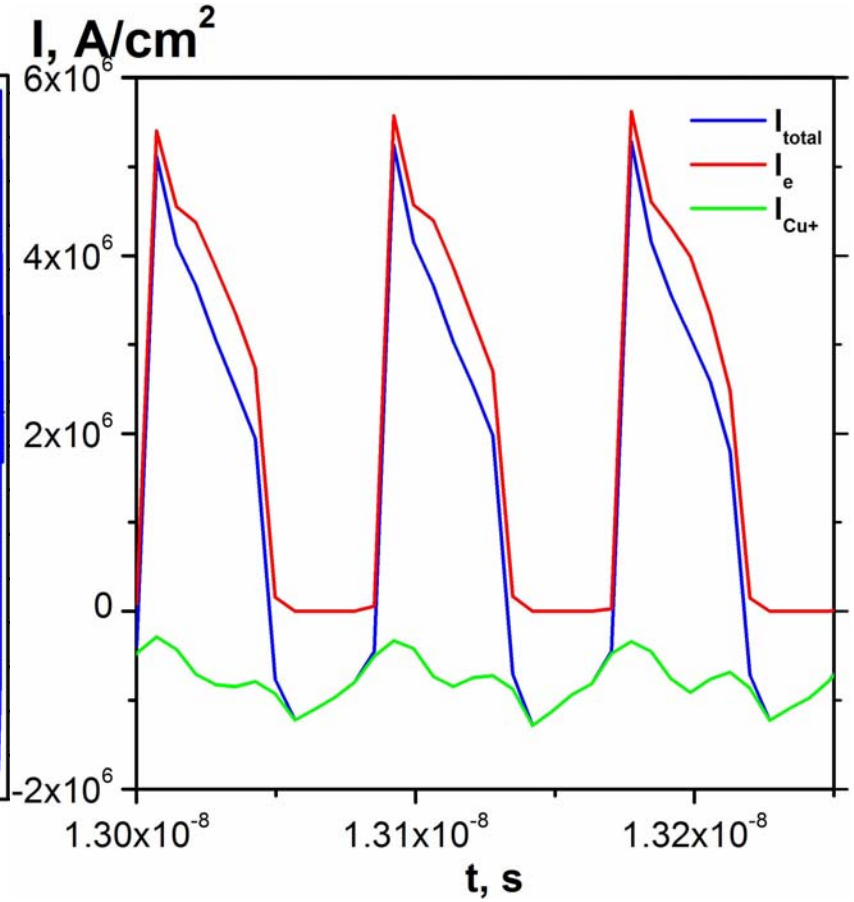
Cu flux energy composition at the powered electrode



PIC modeling of arcing: RF discharge

Discharge current to powered electrode





more results at **http://www.ipp.mpg.de/~knm/CERN/spark2.html**

Towards the integrated modeling of arcing

Particle-in-Cell modeling of arcing

- electric field concentrated in sheath
- triggered by electron field emission
- fluxes of plasma particles increase emission from the electrodes

Integrated Particle-in-Cell and Molecular Dynamics modeling of arcing

- energetic particles create surface damage
- explains experimentally observed cluster emission
- scaling studies on the way
- CERN PhD student position for Helga Timko (starting next year)

Thank you!