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Progress in Breakdown Modelling – MD and PIC Breakdown Simulations

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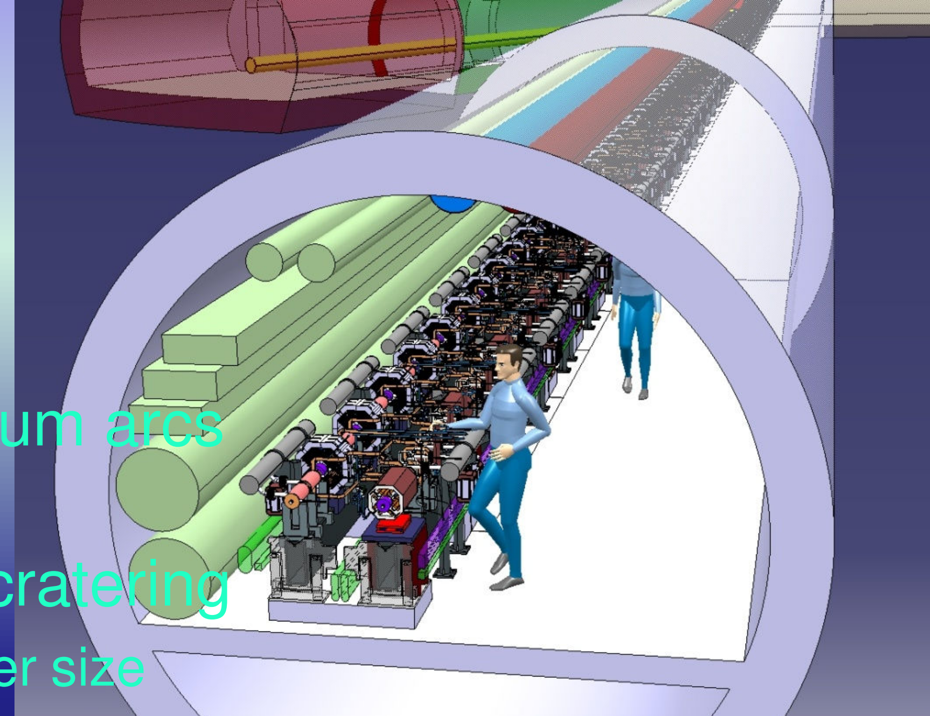
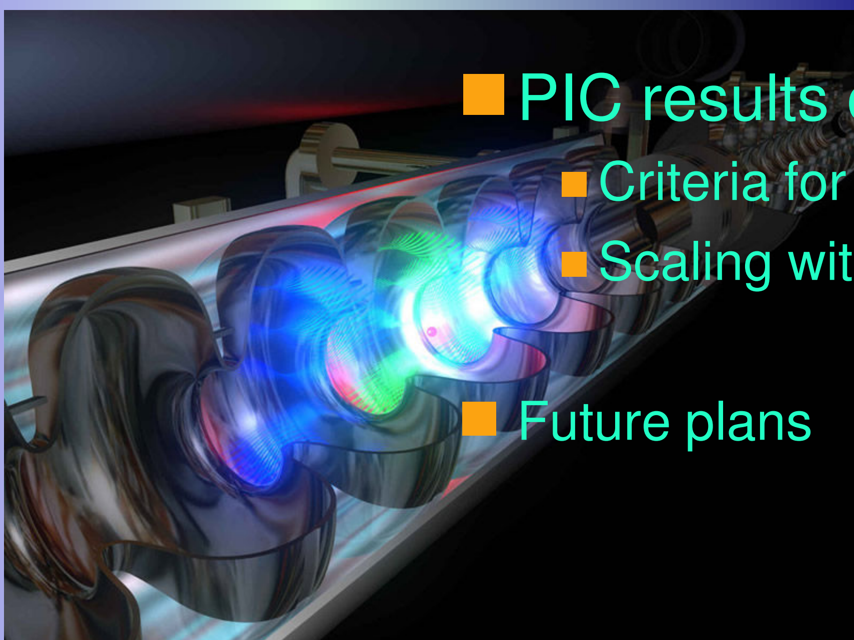
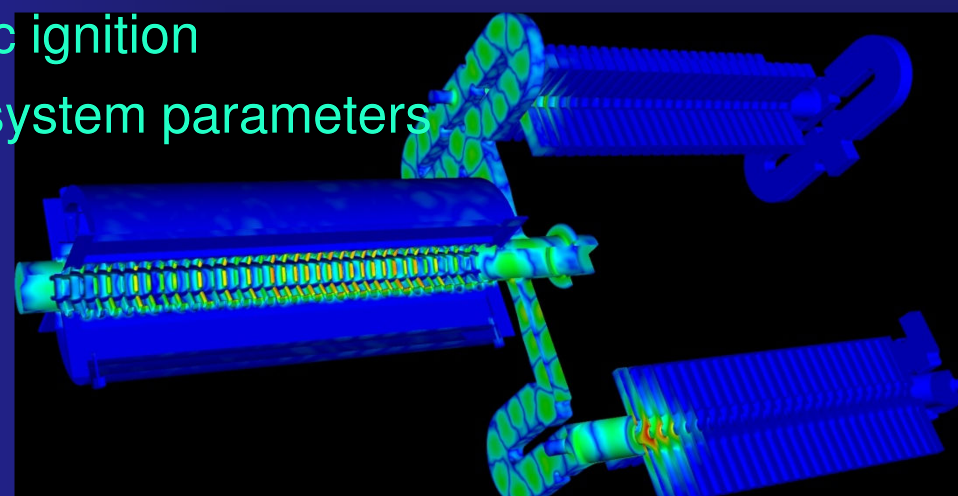
Outline



- Modelling vacuum arcs
- MD results on cratering
  - Scaling of crater size



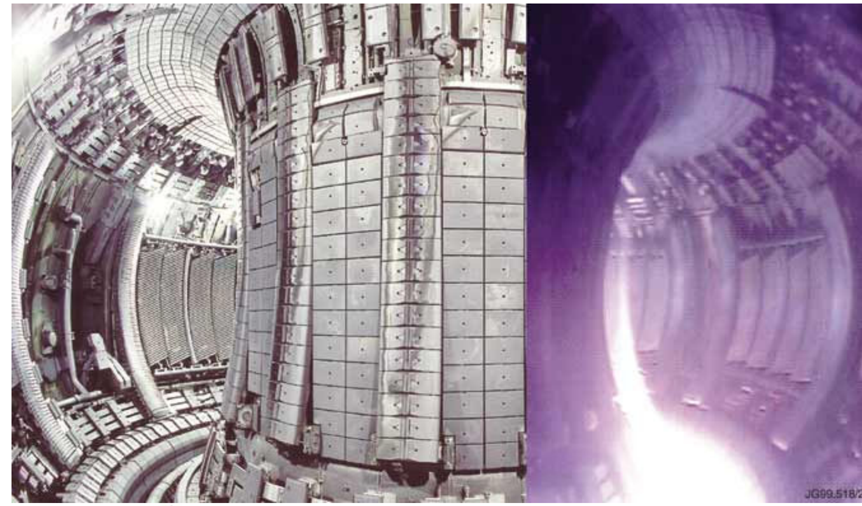
- PIC results on plasma build-up
  - Criteria for arc ignition
  - Scaling with system parameters

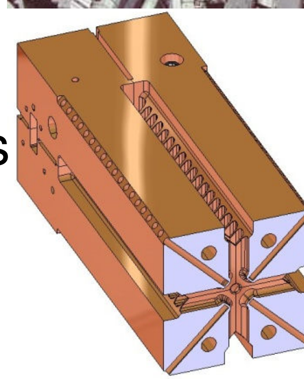


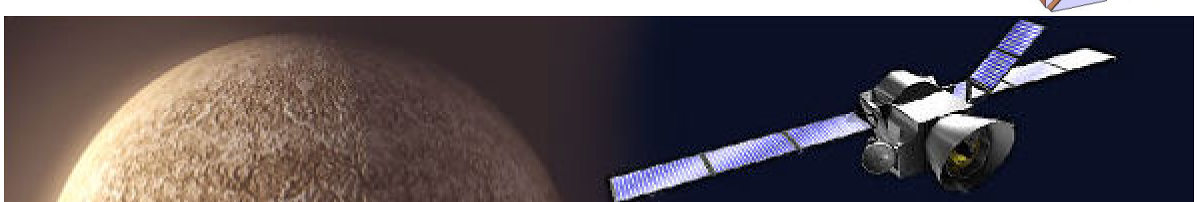
- Future plans

Breakdown studies have a broad application spectrum

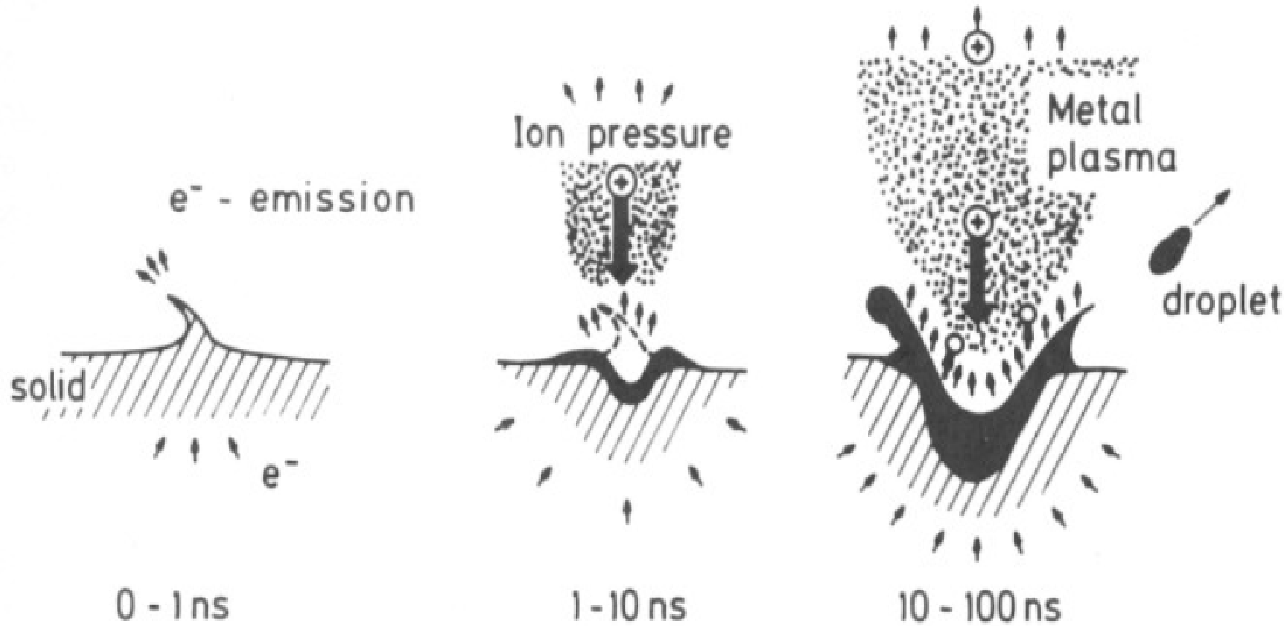
- Fusion physics
- Satellite systems
- Industry
- Linear collider designs







Finally an electric field builds up between the plasma and the surface of the solid named the *Langmuir sheath potential*. Electrical arcs may ignite between the plasma representing the negative electrode and the vessel wall representing the positive electrode.



1. Onset
2. Build-up of plasma
3. Surface damage, new spots

Schematic of the ignition of an electrical arc at a surface tip, as well as burning and movement of the cathode spot [21, 22].

Erosion yields by electrical arcs, in atoms/electron [21],[25]-[30]. The estimated total number of atoms removed for an arc current of 5 to 10 A and a burn time of about 10-100 μs are also introduced.

Multiscale model

Our model corresponds to the above 3 phases.

Stage 0: Onset of tip growth; Dislocation mechanism
Method: MD, Molecular Statics… — ~ sec/min

Stage 1: Charge distribution @ surface
Method: DFT with external electric field — ~few fs

Stage 2: Atomic motion & evaporation
Method: Hybrid ED&MD model — ~few ns

- Classical MD+Electron Dynamics: Joule heating, screening effect
- Solution of Laplace equation

Stage 3: Evolution of surface morphology due to the given charge distribution
Method: Kinetic Monte Carlo — ~ sec/hours

Onset of plasma (Stages 0–3)

=> Electron & ion & cluster emission ions

Stage 4: Plasma evolution, burning of arc
Method: Particle-in-Cell (PIC) — ~10s ns

Plasma build-up

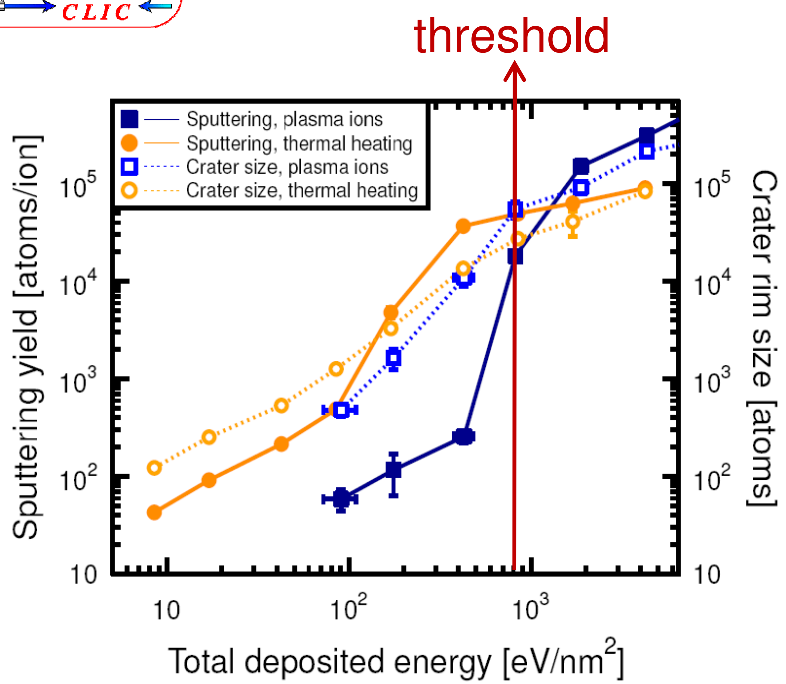
=> Energy & flux of bombarding ions

Stage 5: Surface damage due to the intense ion bombardment from plasma
Method: Arc MD — ~100s ns

Surface damage

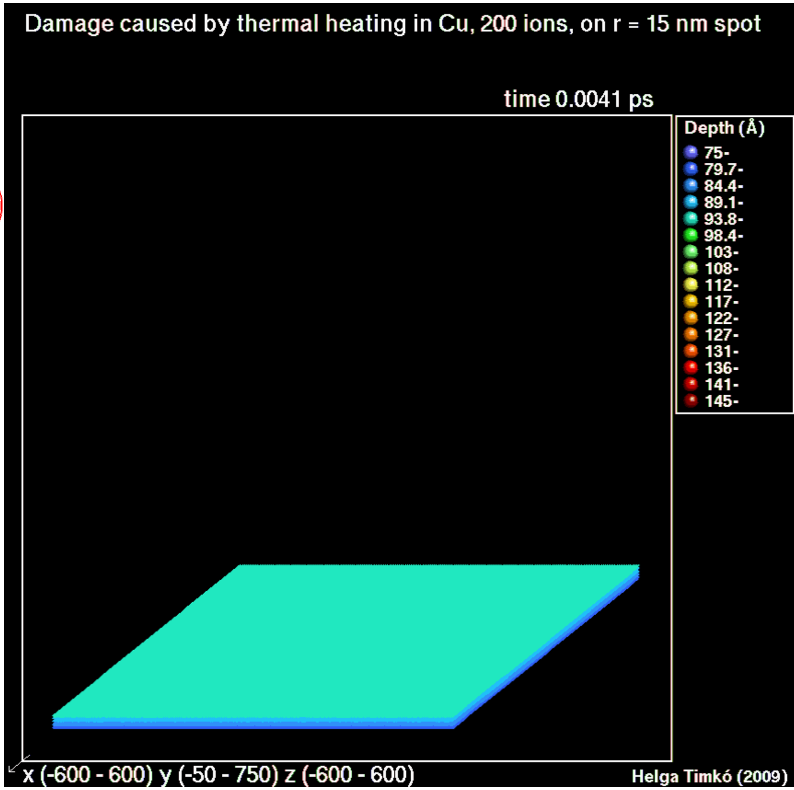
Achievements

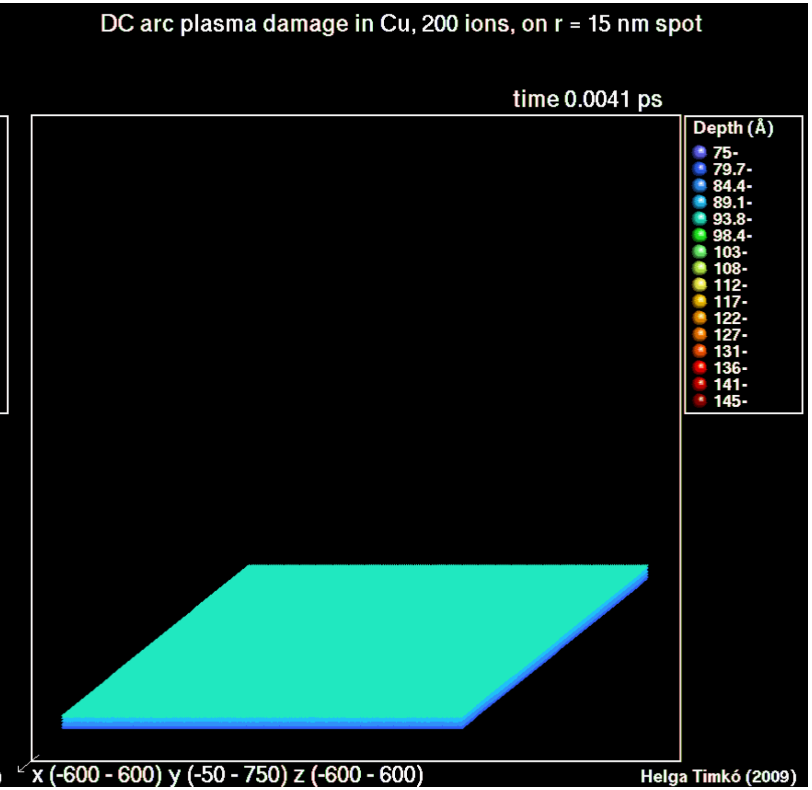
1. Onset: direct field evaporation from surfaces and tips
2. Plasma build-up: we have developed a one-dimensional PIC model and identified plasma build-up criteria
3. Cratering: knowing flux & energy distribution of incident ions, erosion and sputtering was simulated with MD



- Comparing arc plasma bombardment and thermal heating, we found that:
  - Enhanced sputtering yield above a threshold, corresp. to the melting point
  - Only for plasma bombardment:
    (i) heat spike & cluster emission above the threshold
    (ii) experimentally seen complex crater shapes can form

MD simulation of surface damaging

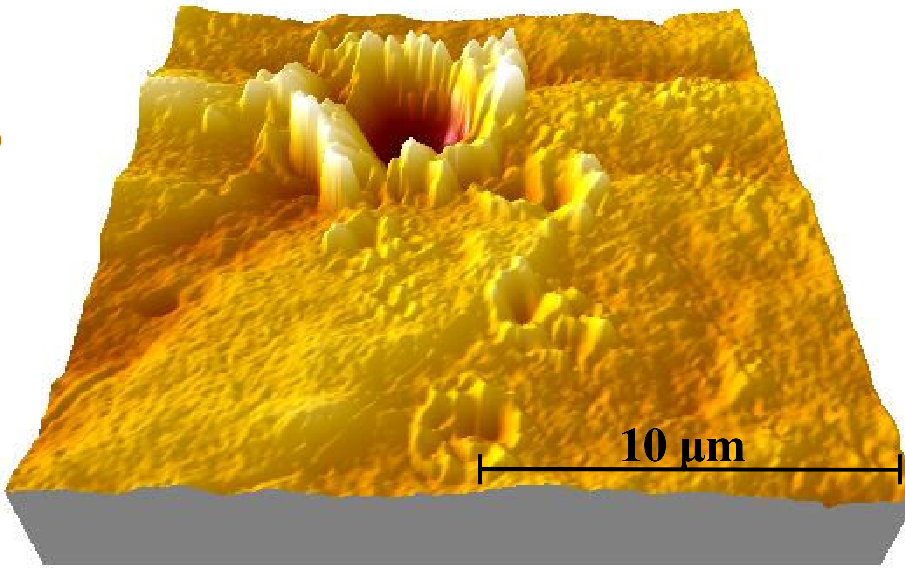


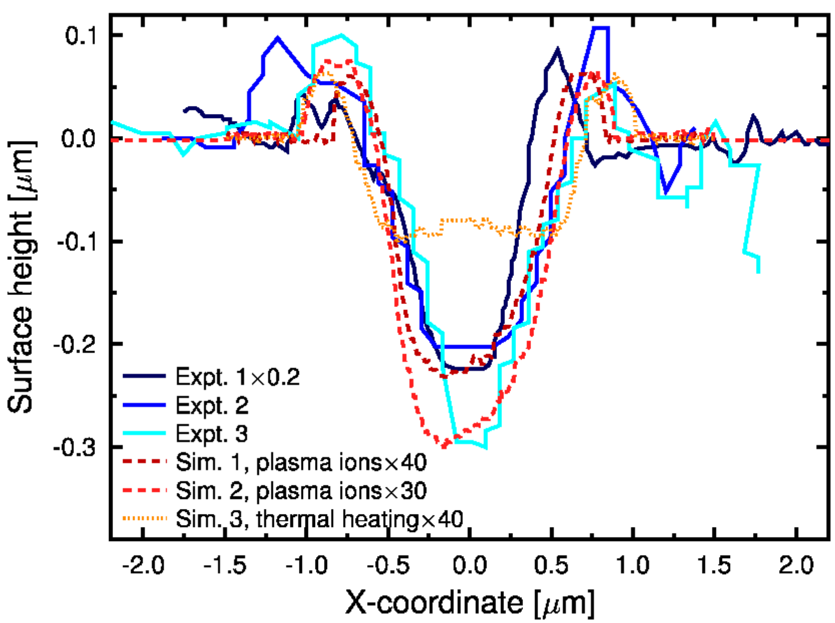


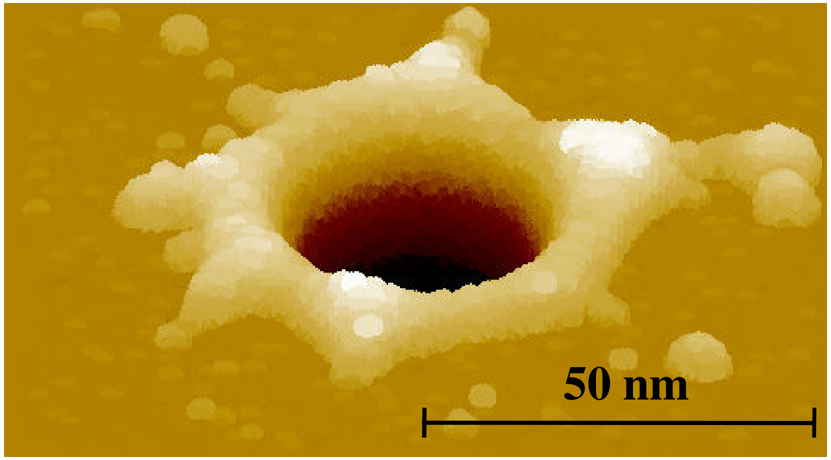
Comparison to experiment

- Self-similarity:

  Crater depth to width ratio remains constant over several orders of magnitude, and is the same for experiment and simulation

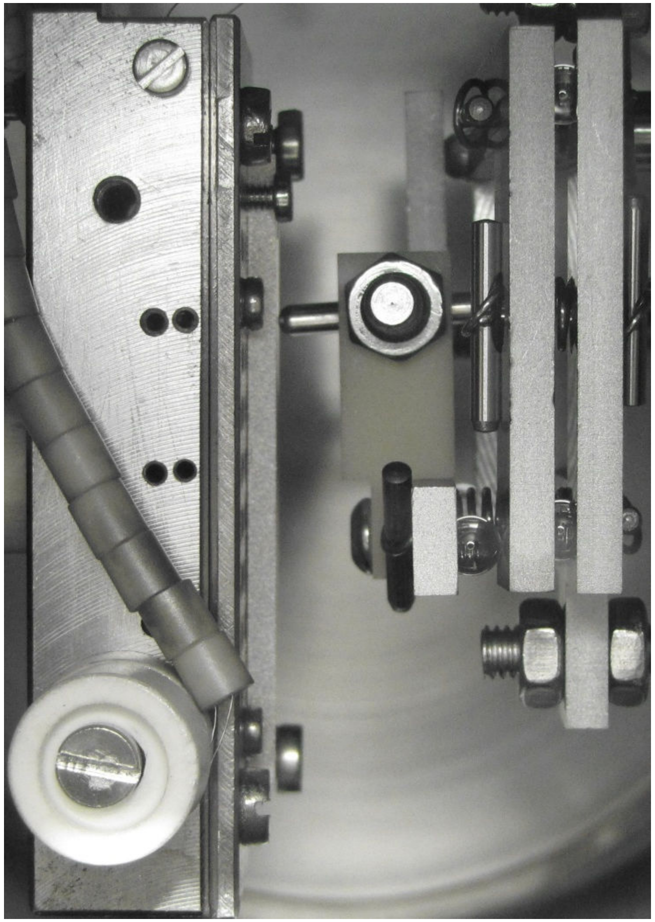






Now to the plasma part…

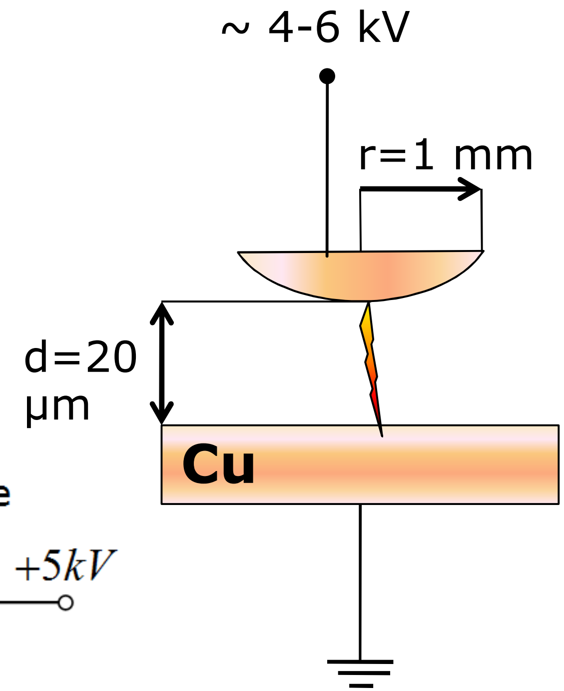
Modelling DC arcs

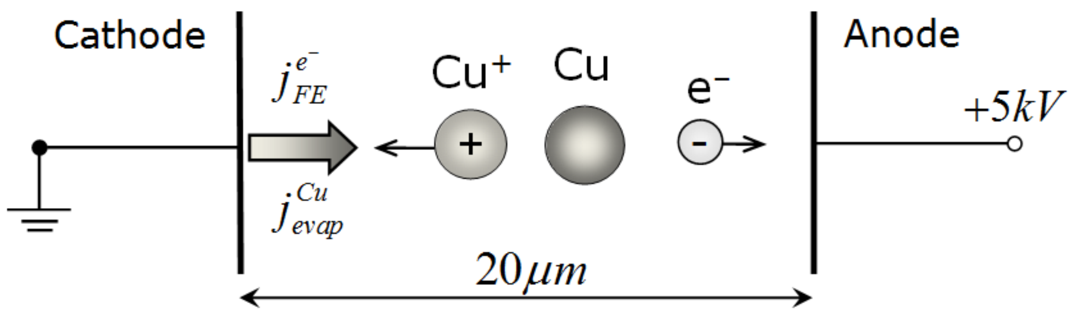


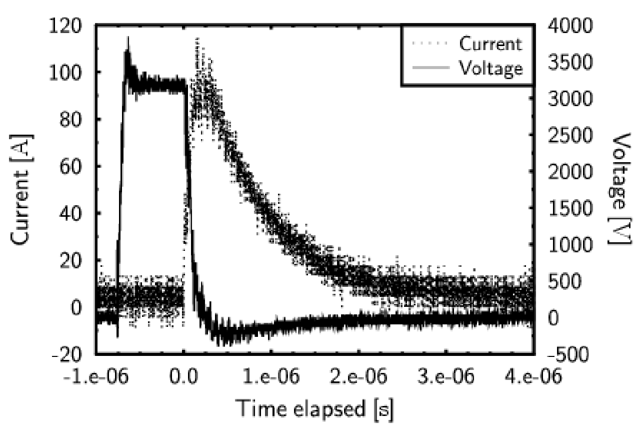
- First we have to understand breakdowns in DC, before we can generalise to RF
- To have a direct comparison with experiments, we adjusted simulation parameters to the DC setup at CERN
- However, the results we present here are completely general and not restricted to the DC setup!

Corresponding to experiment

- 1d3v electrostatic PIC-MCC code
  - Resolving the main stream of plasma
  - Areal densities of physical quantities

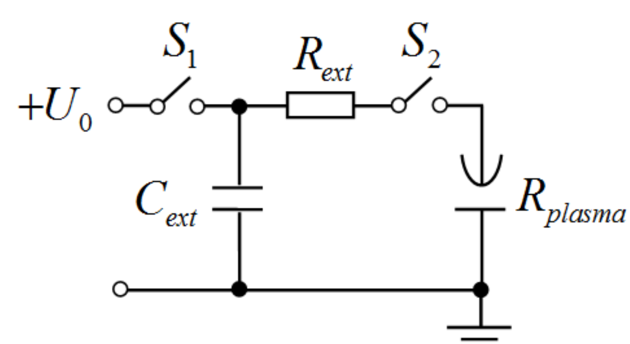






- Exponential voltage drop mimiced
  - Limited energy from the circuit

$$R_{ext} = 30\Omega$$
$$C_{ext} = 0.1 - 27.5nF$$



Phenomena taken into account

We started from a simple model with a code from IPP-MPG

(Collaborators: *R. Schneider, K. Matyash*)

Start from these

- Field emission of electrons, Fowler-Nordheim eq.:

$$j_{FE} = a_{FN} \frac{(eE_{LOC})^2}{\phi t(y)^2} e^{-b_{FN} \frac{\phi^{3/2} v(y)^2}{eE_{loc}}}, \quad \text{where } E_{loc} = \beta \cdot E$$

$$t(y) = 1, \; v(y) = 0.956 - 1.062 y^2 \quad \text{where y=} \sqrt{\frac{e^3 E_{LOC}}{4\pi\varepsilon_0 \phi^2}}$$

- Evaporation of Cu neutrals

Produce ions

- Collisions, esp. ionisation collisions

More e- & Cu

- Sputtering of Cu neutrals at the wall
- Secondary electron yield due to ion bombardment

Plasma build-up from a field emitter tip

- We start from a field emitter tip → supply of electrons and neutrals → build-up of plasma
- The *field emitter* is assumed in terms of an initial field enhancement factor
  - Dynamic beta: the ”erosion” and the ”melting” of the tip was implemented
  - We define the ”melting current” j_{melt} as the threshold of electron emission current, which, if exceeded, sets β=1
- *Neutral evaporation*: an estimate was needed
  - Define the neutral evaporation to electron FE ratio $r_{Cu/e} = r_{Cu/e}(E,t,\ldots)$ and approximate it with a constant

Under what conditions will an arc form?

Two conditions need to be fulfilled:

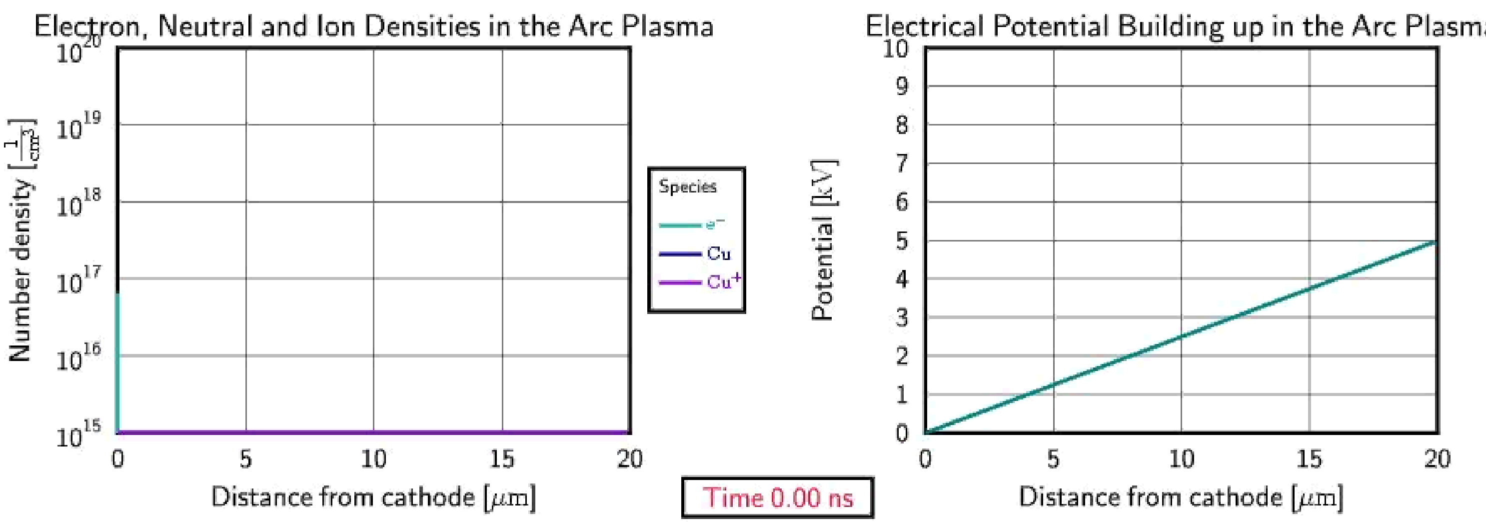
- High enough **initial local field** to have growing FE current
- Reaching the **critical neutral density** to induce an ionisation avalanche

- The sequence of events leading to plasma formation:
  - Due to high electric field: electron FE, neutral evaporation
  - Ionisation and acceleration of the charged particles

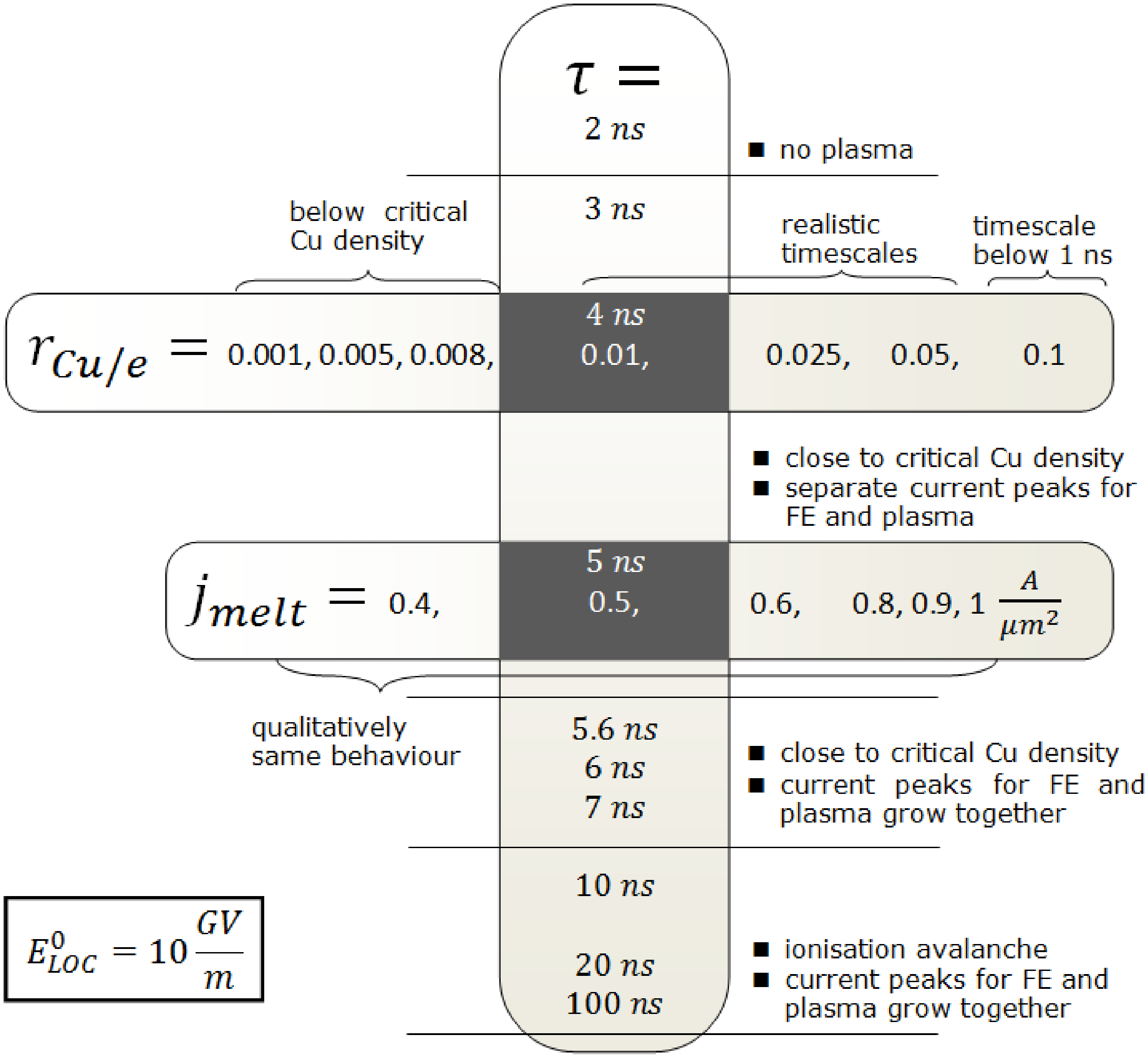
    $\Rightarrow$ e^-, Cu and Cu^+ densities build up
  - "Point of no return": $l_{mfp} < l_{sys}$ – corresponding to a critical neutral density ~ 10^{18} $1/cm^3$ in our case
  - Ions $\rightarrow$ sputtering neutrals $\rightarrow$ more ions $\Rightarrow$ ionisation avalanche

Plasma build-up

The only limiting parameter is what power can be supplied to the arc



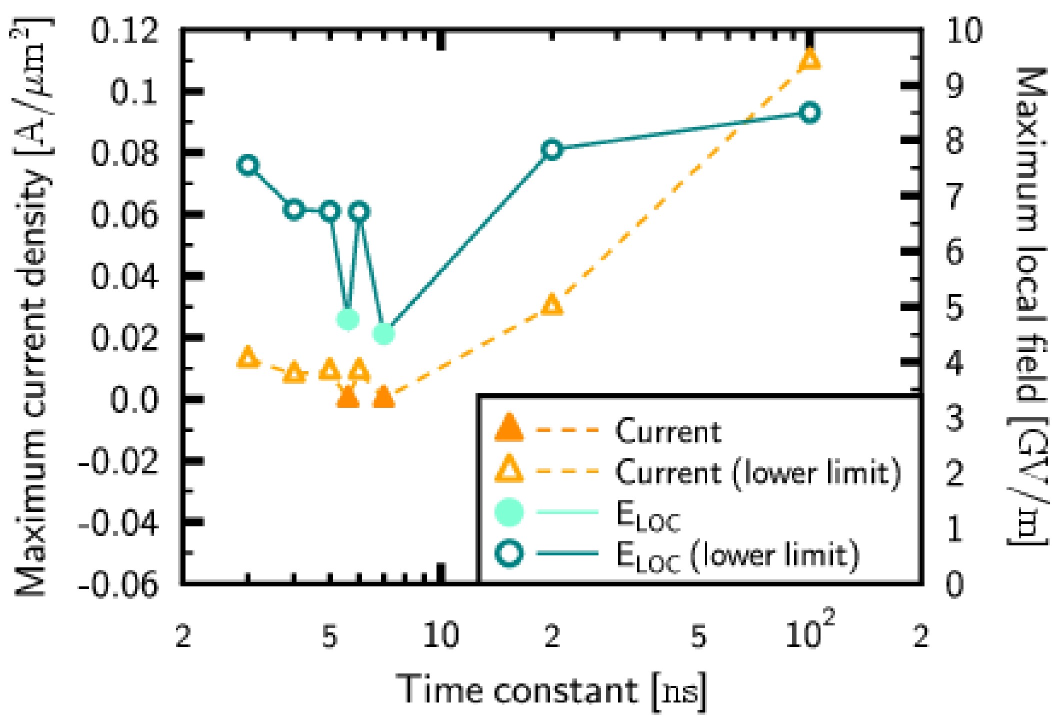
Parameter space investigated



$$E_{LOC}^{0} = 10 \frac{GV}{m}$$

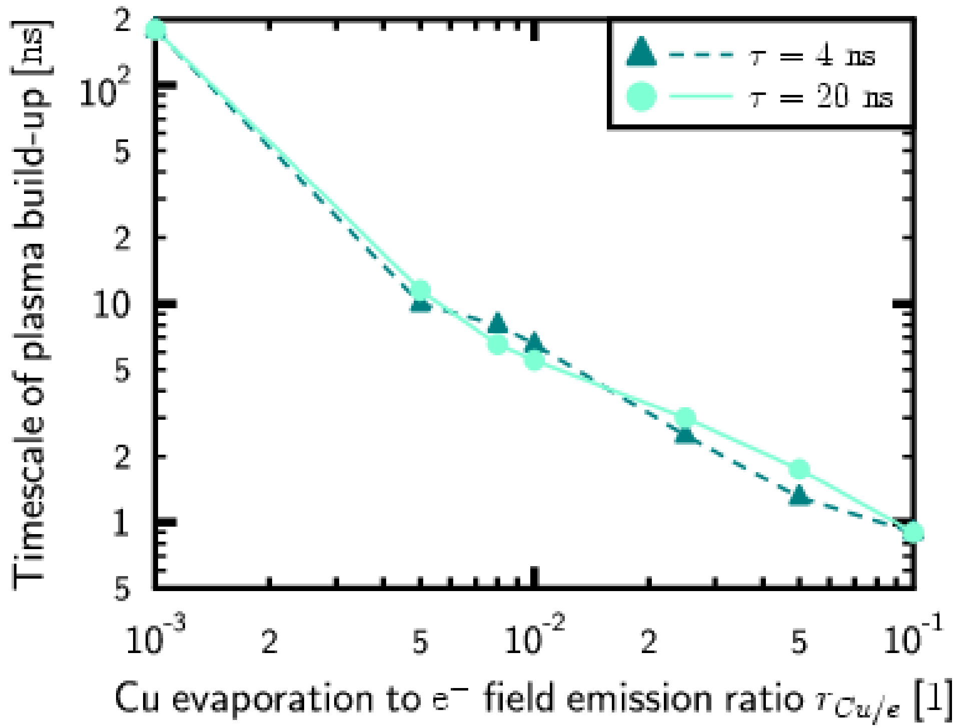
Time constant

- Close to critical Cu density below ~ 10 ns
- Above ~ 10 ns, plasma formation is unavoidable



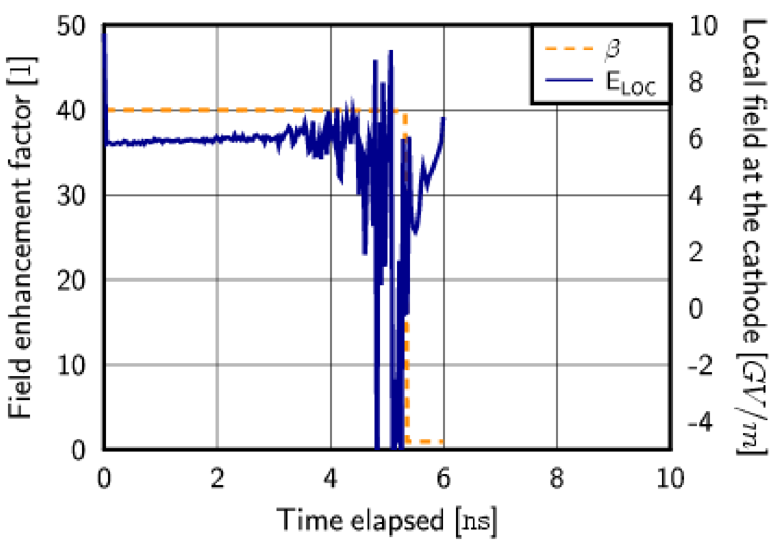
Neutral evaporation to electron FE ratio

- 0,001 – 0,008: below critical Cu density
- 0,01 – 0,05 gives realistic timescales for plasma build-up



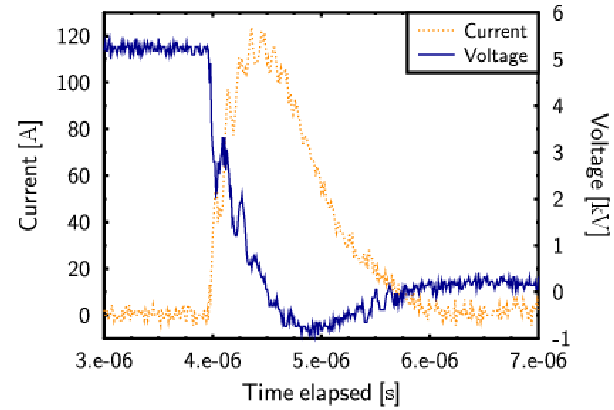
Initial local field required

- Up to now, 10 GV/m was assumed (measured value)
- Lowering E_{LOC} (either β or E) gave drastical changes
  - 8 MV/m: no ionisation avalanche any more
  - 7.5 MV/m and lower: no plasma at all

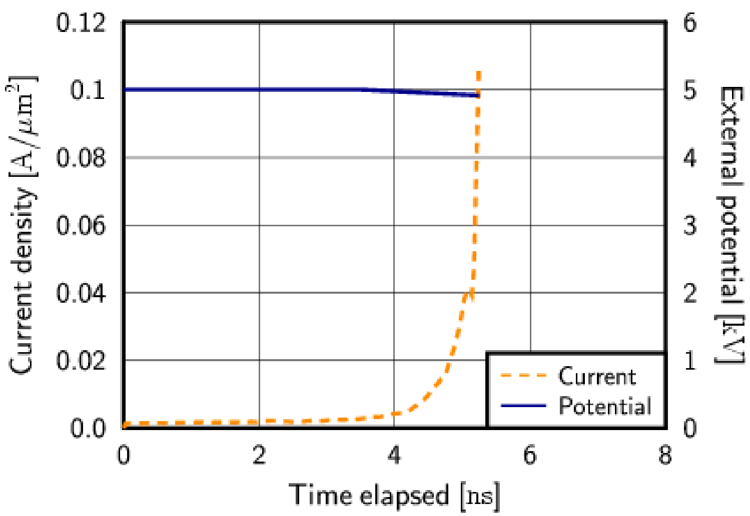


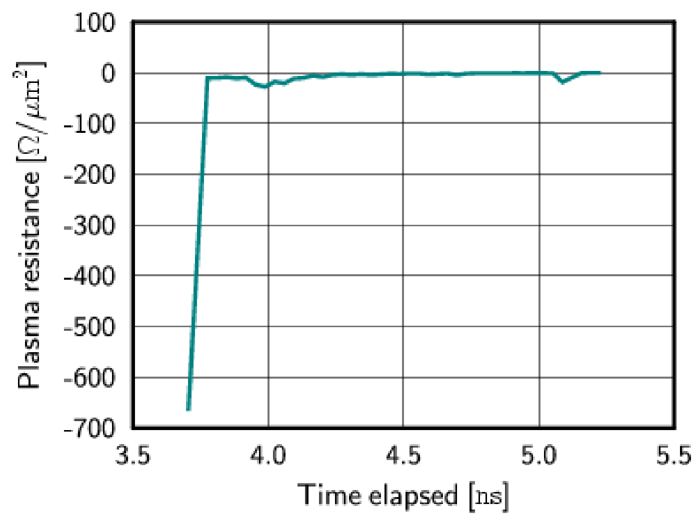
- The criterion seems to be:
  to stabilise around ~6 GV/m to get growing FE current
- What happens if E_{LOC} = 12 GV/m?
  - It also stabilises to 6 GV/m only!
  - Note: BDR = 1 reached

Circuit characteristics



- Plasma has negative resistance
- The plasma seems to match the impedance of the external circuit to consume the available energy in the most effective way



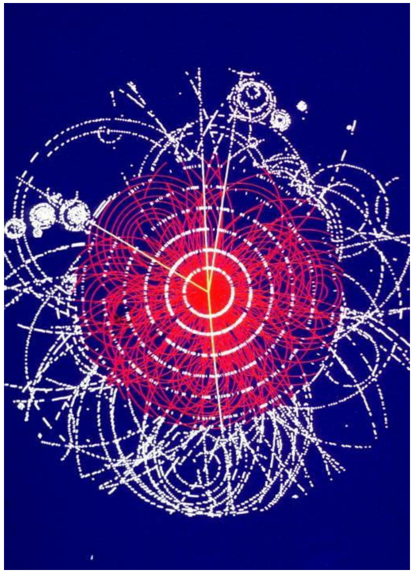


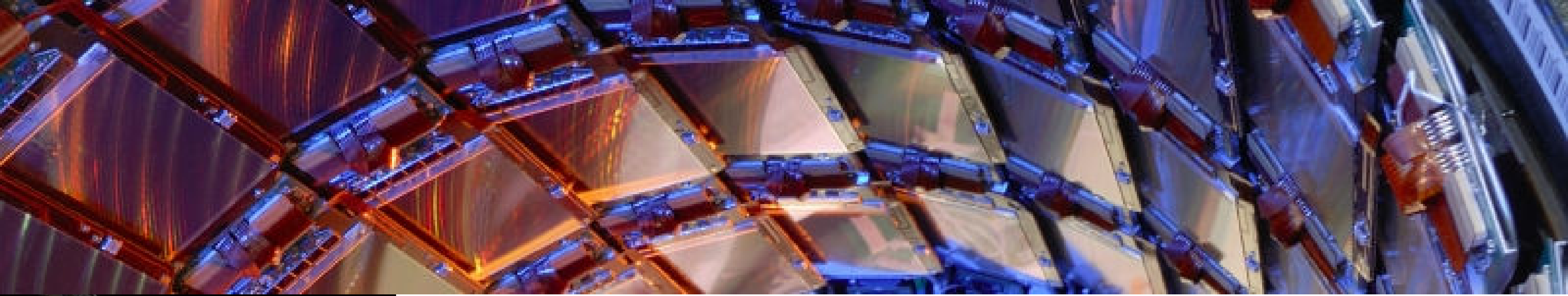
Conclusions of the 1D model

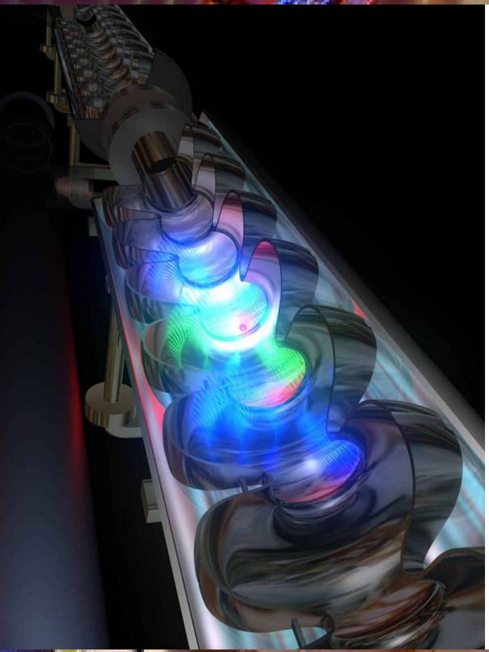
- When the 2 required conditions (high enough initial local field, reaching the critical Cu density) are fulfilled, plasma formation is inevitable
- The 1D model is suitable to obtain information on fluxes, densities etc. in the main stream of the plasma
  - Restricted to the build-up phase of plasma
- Also RF can be simulated, requires only minimal modifications in the code

Future plans

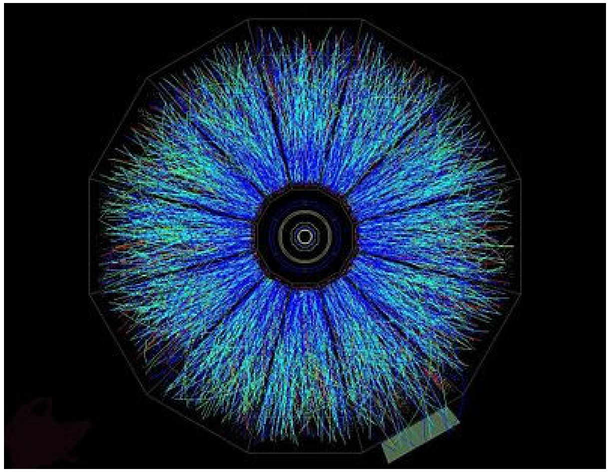
- Extension to a 2D model; we gain:
  - Information on the radial distribution and diffusion of the plasma
  - Resolving area
  - Self-consistent PIC-MD coupling
  - Self-consistent coupling between the external circuit & discharge gap
- Then we could build in also more easily
  - Thermionic emission
  - SEE
- Investigation of RF and other materials







Thank you!

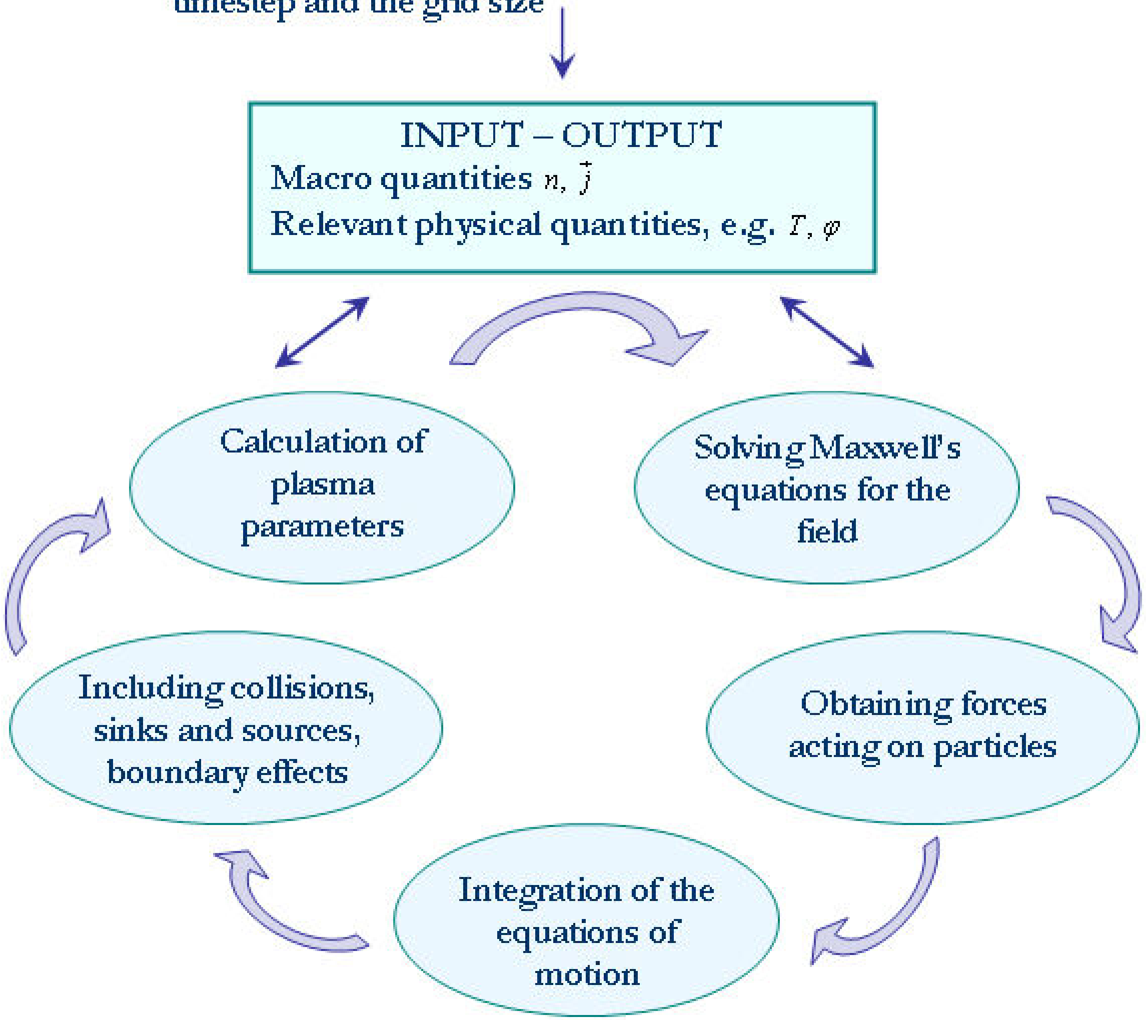


Back-up slides

The Particle-in-Cell method

Setting up the simulation:

Defining superparticles, reference values, boundary conditions, timestep and the grid size



The Particle-in-Cell method

- Basic idea: simulate the time evolution of *macro quantities* instead of particle position and velocity (cf. MD method)
  - Fields and forces calculated on the grid
  - Superparticles
  - Restricted to certain regime of number density (ref. values)
  - Kinetic approach of plasma, but can be applied both for collisionless and collisional plasmas
- Application fields: solid state physics, quantum physics…
- Has become very popular in plasma physical applications
  - Esp. for modelling fusion reactor plasmas (sheath and edge)

- In our application:
  - 1D code (no side losses resolved)
  - Electrostatic: only Poisson's eq.

$$\frac{\varphi_{i+1} - 2\varphi_i + \varphi_{i-1}}{(\Delta x)^2} = -\frac{\rho}{\varepsilon_0}.$$

I. Field emission, neutral evapotation

- Dynamic electron field emission current according to FN
  - Space charge corrections: Above 0.6 A/μm^2
  - PIC takes into account both the external+internal potential, so this is taken automatically care of
  - Thermionic emission can not be incorporated into 1D
- Beta expected to vary too; a dynamic beta, the ”erosion” and the ”melting” of the tip was implemented
  - We define the ”melting current” j_{melt} as the threshold of electron emission current, which, if exceeded, sets β=1
- Neutral evaporation: An estimate was needed
  - Define the neutral evaporation to electron FE ratio $r_{Cu/e}$ = $r_{Cu/e}$(E,t,…) and approximate it with a constant
  - What is the possible range of $r_{Cu/e}$?

II. Collisions

With PIC we are limited in dynamic range/highest density that can be simulated; restricts to plasma build-up phase

⇒ We treat only three species: e^-, Cu and Cu^+

- Coulomb colisions for all possible pairs,

$$(e^-, e^-),\ (e^-, Cu^+)\ \text{and}\ (Cu^+, Cu^+)$$

- Electron-neutral elastic collisions

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

- Neutral-neutral elastic collisions

$$Cu + Cu \rightarrow Cu + Cu$$

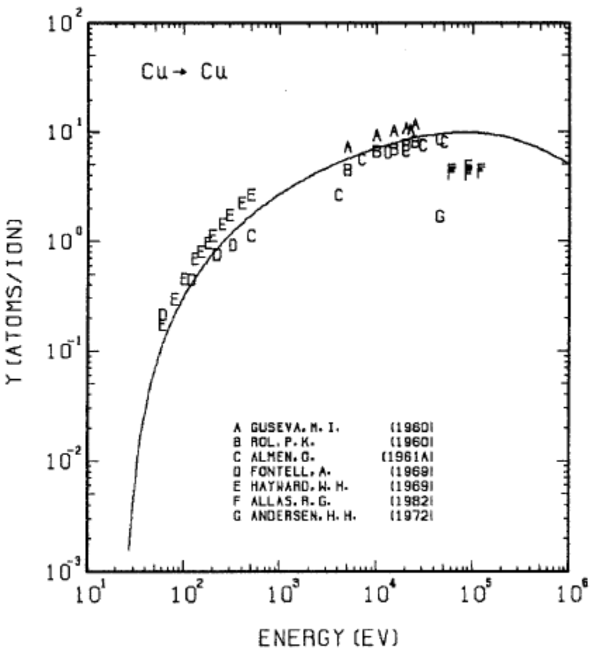
- Electron impact ionisation

$$e^- + Cu \rightarrow 2e^- + Cu^+$$

- Charge exchange and momentum transfer

$$Cu^+ + Cu \rightarrow Cu^+ + Cu$$

III. Surface interaction model



[Yamamura & Tawara]

- Neutrals and ions sputter neutrals at the walls
  - Energy dependent experimental yield
- Ions bombarding the cathode have in addition
  - An enhaced sputtering yield when the ion flux is above a given threshold (based on MD simulations)
  - A constant SEY = 0,5
  - SEE not yet included, but was implicitly parametrised through testing high SEY