A Review on CLIC Breakdown Studies

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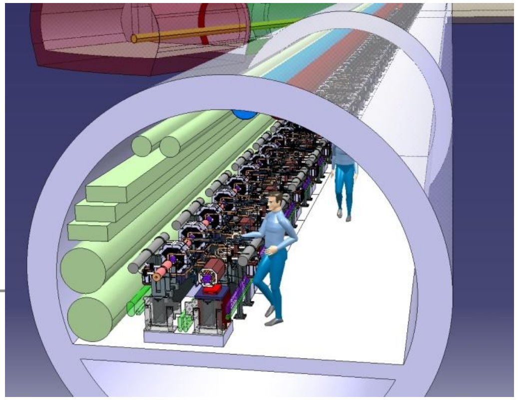
In collaboration with the Max-Planck Institut für Plasmaphysik

Outline

- Why to model vacuum discharges?
  - Compact Linear Collider and others
- Experiments at CERN
  - RF and DC breakdowns
- Theory: A multiscale model
  - Tip growth
  - Plasma formation
  - Surface damage

Helga Timkó

Main concern: Vacuum discharges in CLIC

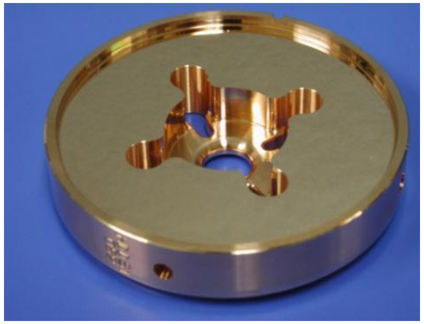


- Why to study vacuum discharges?

1. Going to the limits of conventional acceleration techniques → *highest possible gradient*
2. Estimated power consumption: **415 MW** (LHC: 120 MW) → *cost reduction by efficiency optimisation*

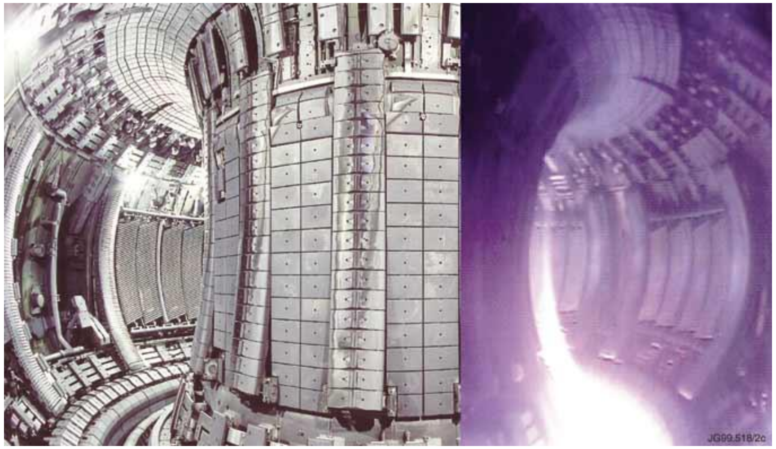
- Knowing how to lower breakdown rate is a key issue in points (1) and (2)

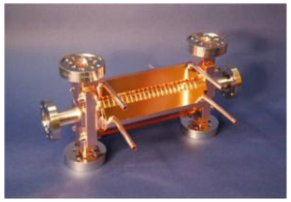
Detail of a CLIC accelerating structure, working at 100 MV/m

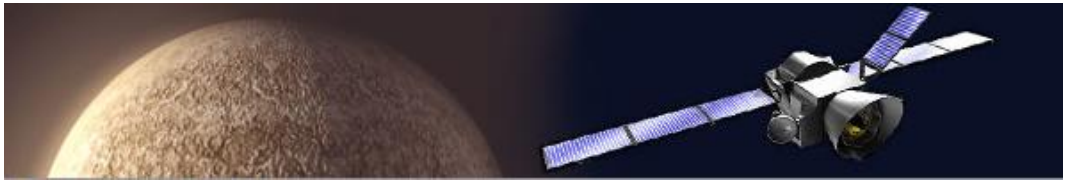


Breakdown studies have a broad application spectrum

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







Issues about breakdown

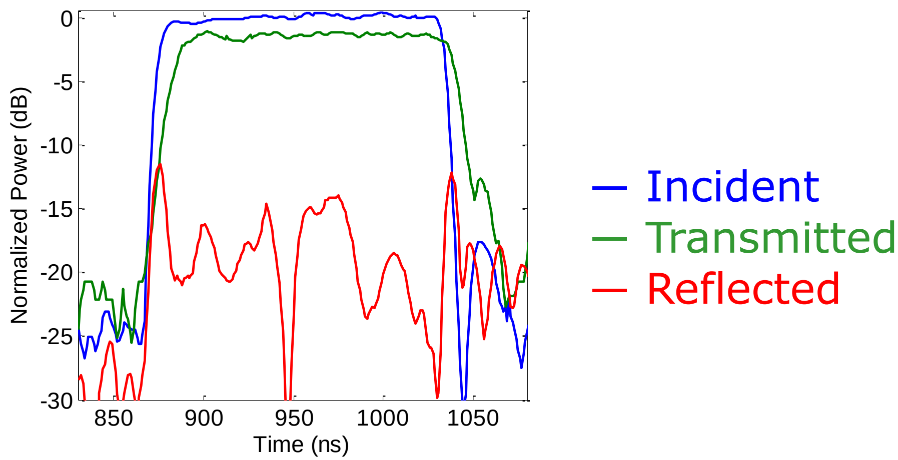
Aim: Predict already in the design phase what breakdown behaviour a structure will have! *Why this is not trivial:*

- Lowering breakdown rate (BDR)
  - How to prevent breakdowns? = How are they triggered?
- Better understanding BDR to predict structure behaviour
  - Statistical or deterministic, independent events or "memory"?
  - Influence of material properties, surface treatments?
- Interpreting measurements – benchmark against theory; *why this is not easy:*
  - Involves many areas of physics
  - Different phenomena are interacting in a complicated way, involving time scales ~fs – h and length scales ~nm – m
  - Non-linear evolution of processes

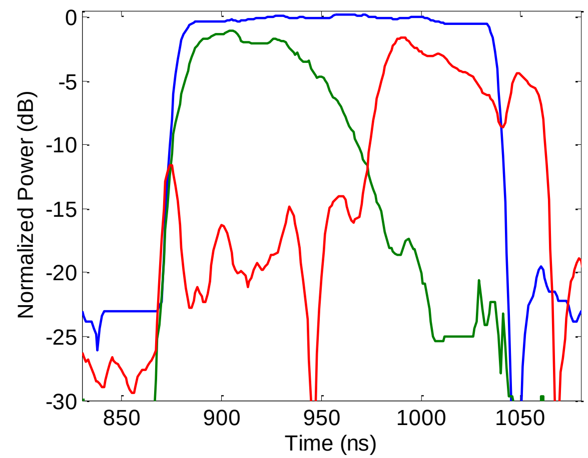
Breakdown Experiments

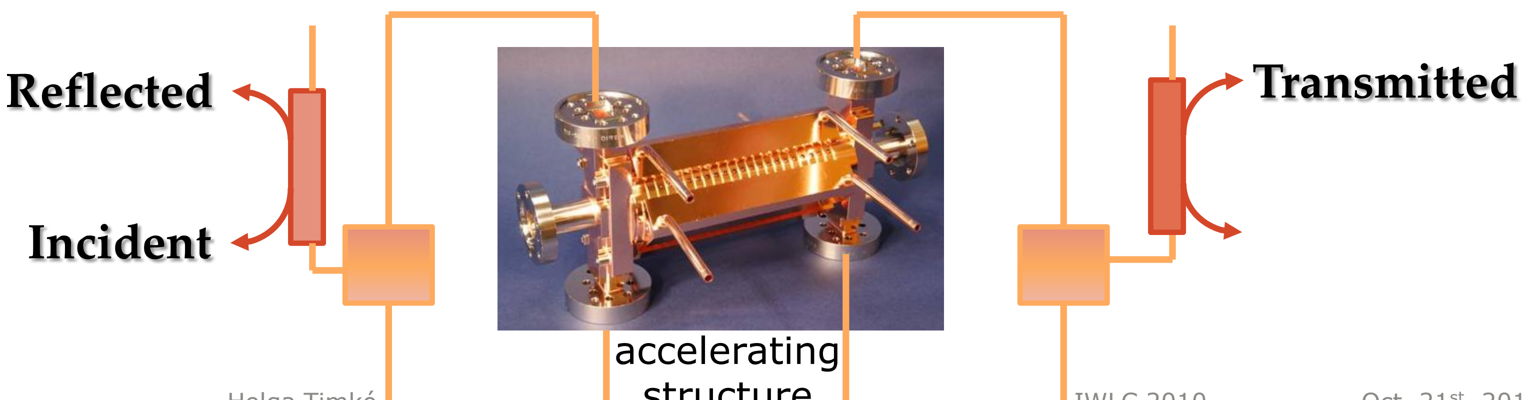
Breakdowns in RF cavities – and how to diagnose them

- Normal waveform



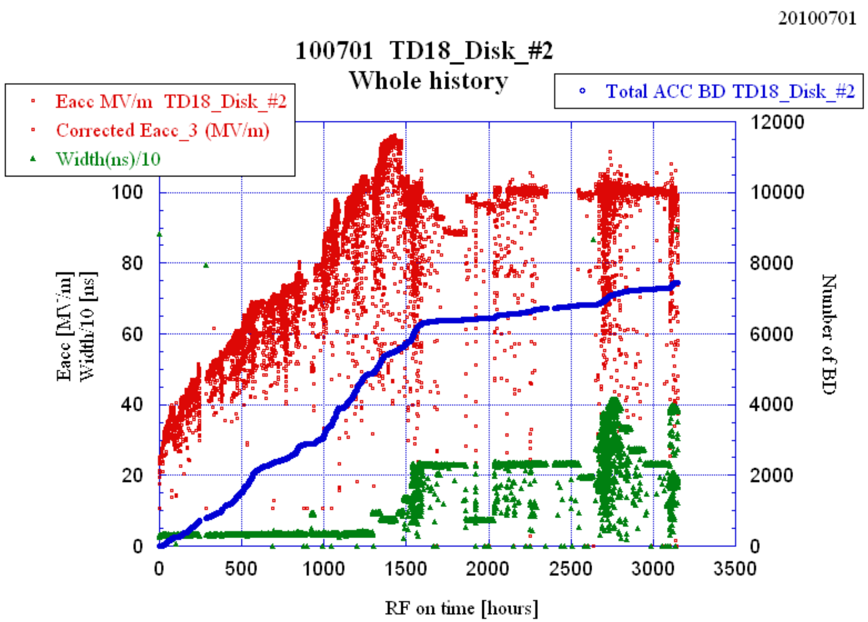
- Breakdown waveform

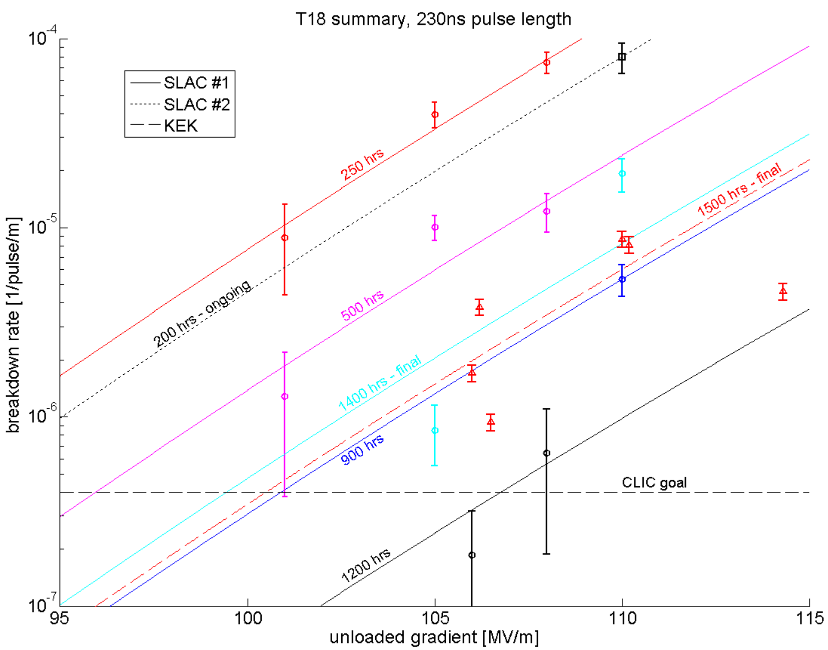




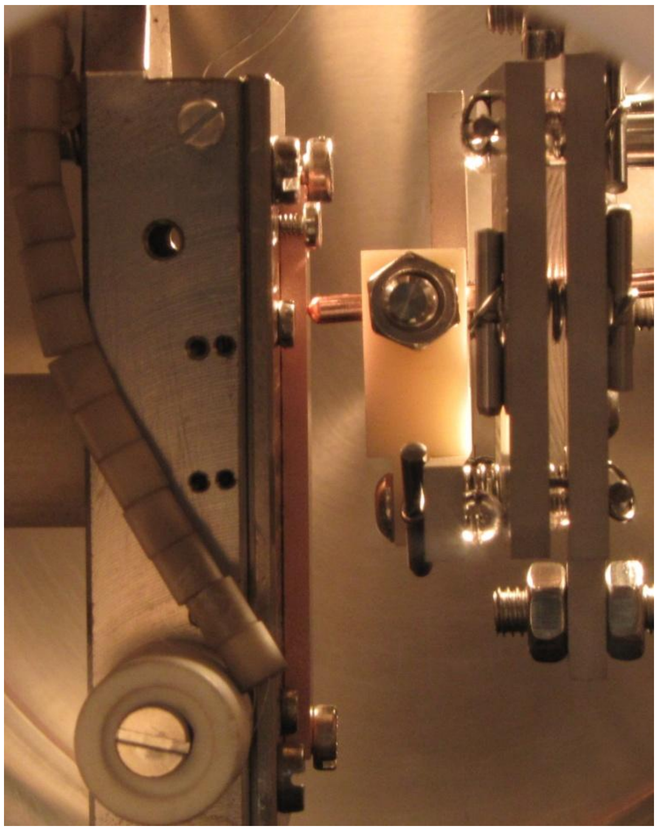
Some open questions...

- What is the physics behind conditioning?
- How does BDR w.r.t. gradient scale and why?



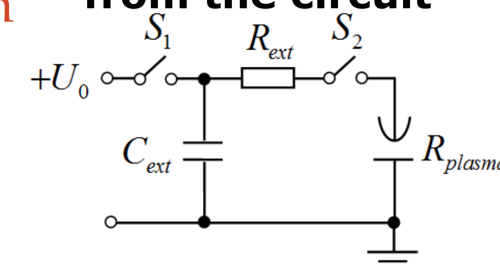


Modelling DC discharges



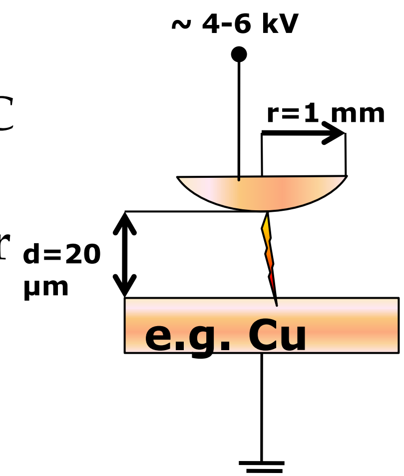
- First we have to understand breakdowns in DC, before we can generalise to RF
- Simple and cost-efficient testing of breakdown behaviour with two *DC setups at CERN*
  - We adjusted also out theoretical model to the DC experimental conditions
- How do we know, whether and how results are valid in RF?

Limited energy from the circuit



$R_{ext} = 30\Omega$

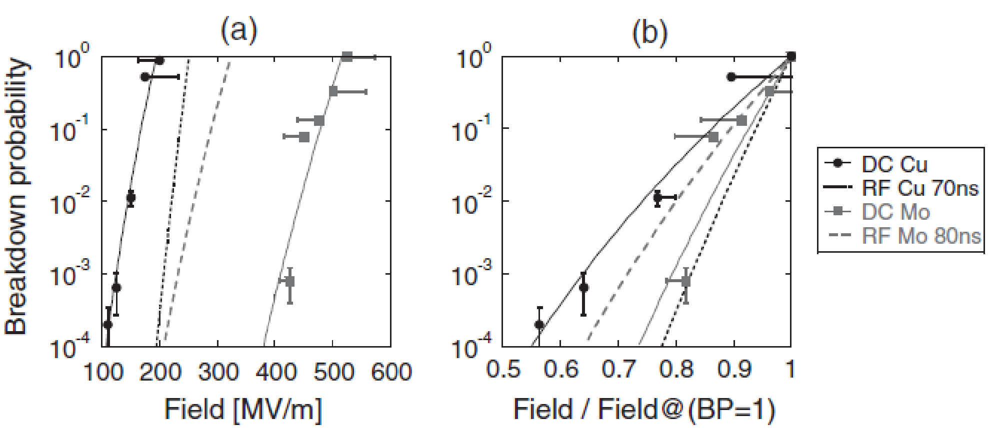
$C_{ext} = 0.1 - 27.5nF$

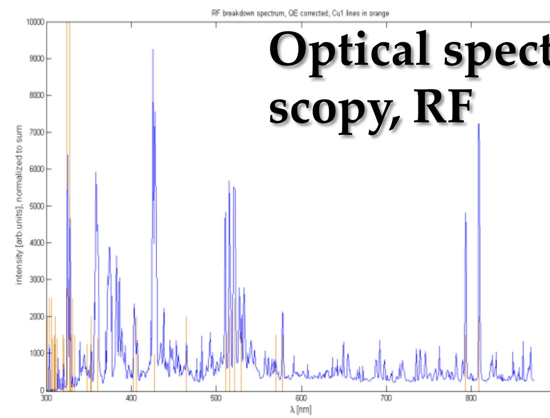


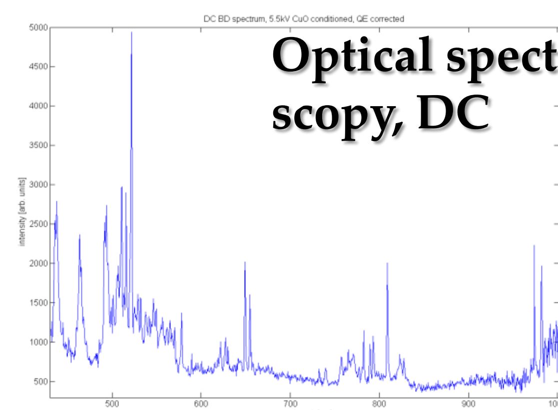
Connection between DC and RF?

- Connection indicated both by theory and experiments; but *how to relate them?*

BDR vs gradient in DC and RF:
Despite all differences in the experimental setup, slopes are almost the same

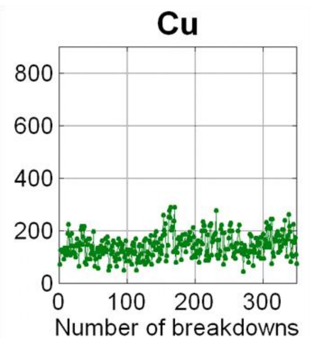




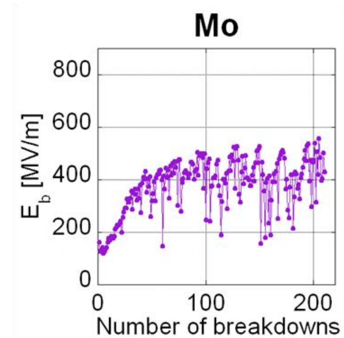


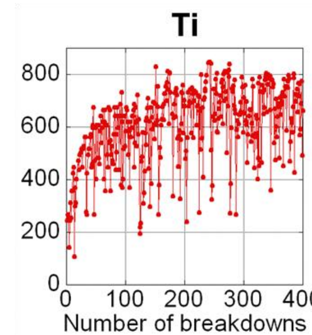
Courtesy of J. Kovermann

Conditioning and ranking of materials

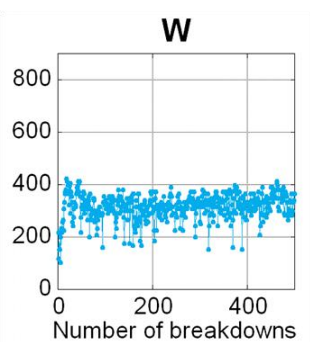


- Also in DC, materials exhibit conditioning, although differently as in RF. *Connection between them?*

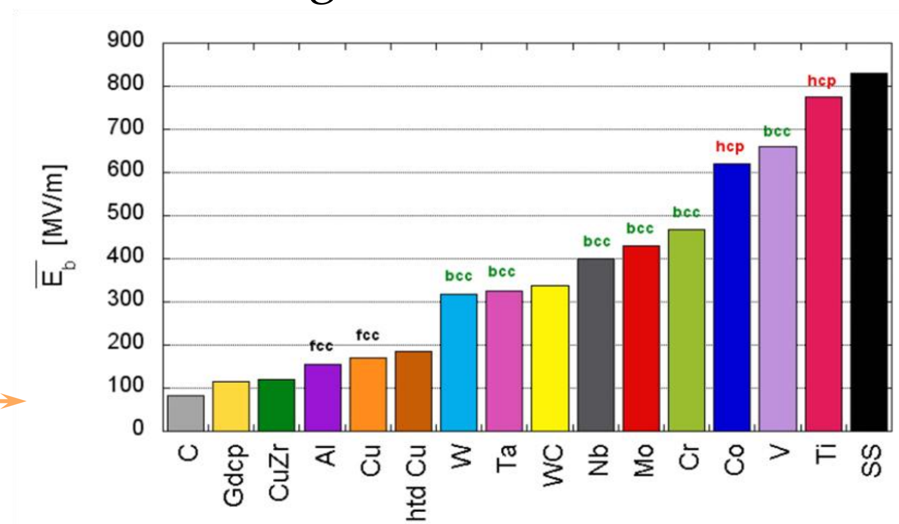




- Ranking of materials according to their breakdown field reached after

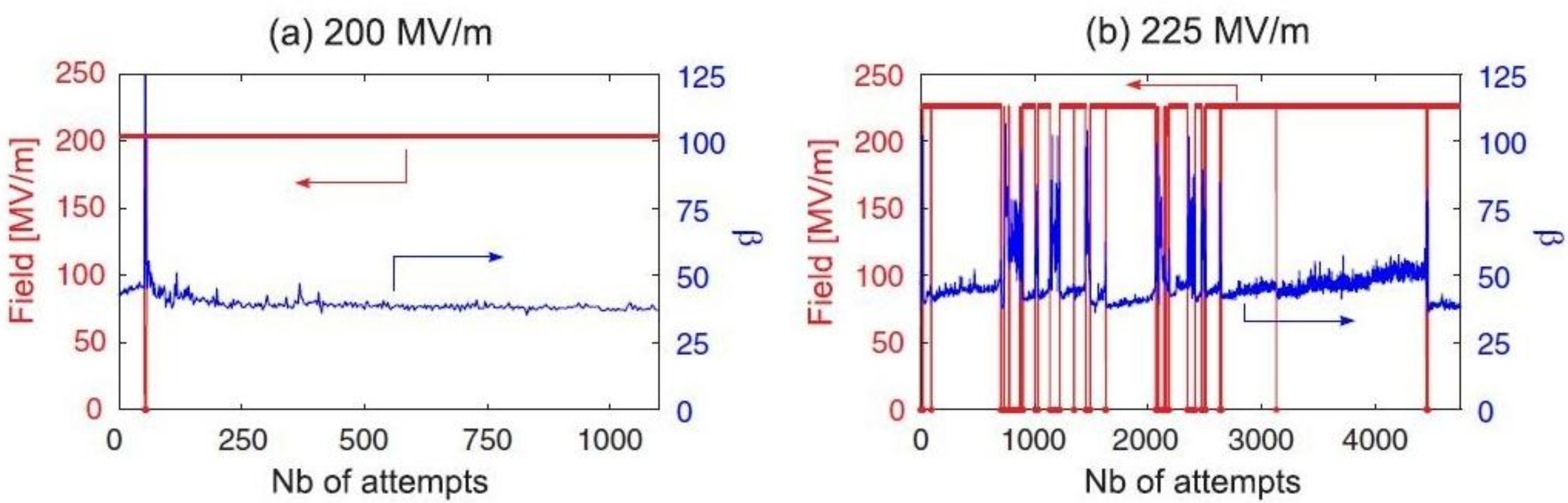


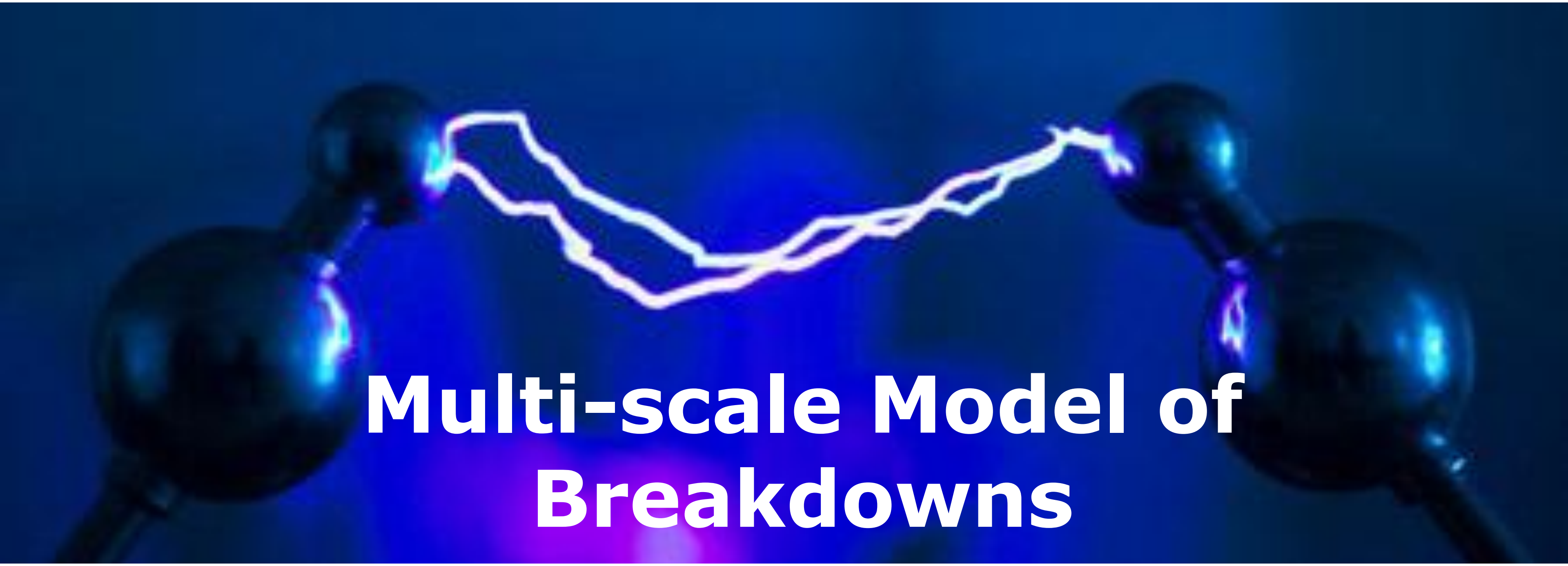
Determined by lattice structure?



An evolving field enhancement?

- Does repeated application of the field modify the surface?





Multi-scale Model of Breakdowns

Electrical breakdown in multi-scale modeling approach

Kai Nordlund, Flyura Djurabekova

Avaz Ruzibaev — Stage 1: Charge distribution at the surface
Method: DFT with external electric field
~few fs

Flyura Djurabekova — Stage 2: Atomic motion & evaporation ;
Joule heating (electron dynamics)
Method: Hybrid ED&MD model (includes Laplace and heat equation solutions)
~few ns

~ sec/min — Aarne Pohjonen — Stage 3a: Onset of tip growth;
Dislocation mechanism
Method: MD, analysis of dislocations

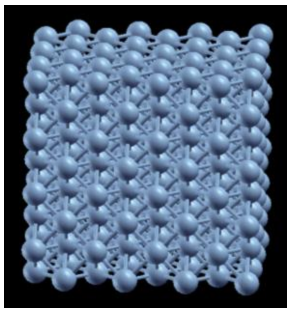
Stefan Parviainen — ~ sec/hours — Stage 3b: Evolution of surface morphology due to the given charge distribution
Method: Kinetic Monte Carlo

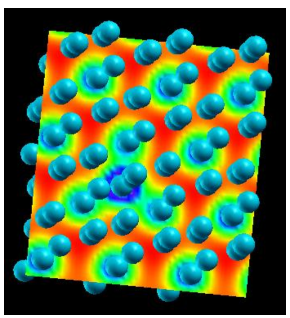
Helga Timkó — Stage 4: Plasma evolution, burning of arc
Method: Particle-in-Cell (PIC)
~10s ns

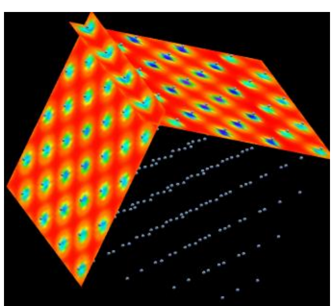
Juha Samela
Leila Costelle — Stage 5: Surface damage due to the intense ion bombardment from plasma
Method: Arc MD
~100s ns

PLASMA ONSET

Stage 1: DFT Method for charge distribution in Cu crystal



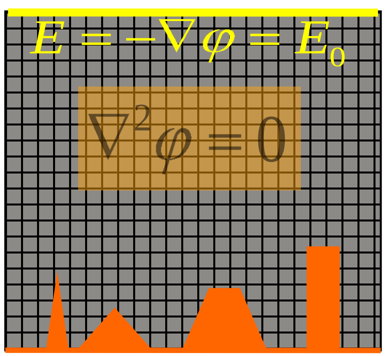




- Writing the total energy as a functional of the electron density we can obtain the ground state energy by minimizing it.
- This information will give us the properties of Cu surface
  - Total energy, charge states (as defect energy levels)
- The calculations are done by SIESTA (Spanish initiative for electronic structure with thousands of atom)
- The code allows for including an external electric field
- The surface charges under the field are analyzed using the Mulliken and Bader charge analysis

Stage 2: Hybrid ED&MD – Partial surface charge induced by an external electric field

Laplace solver

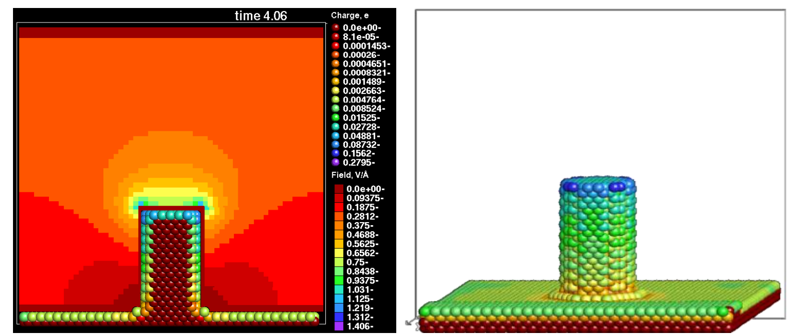


φ=const
(conductive material)

- Standard MD solving Newton's eqs.
- Gauss' law → charge of surface atoms $\sigma = \varepsilon_0 F_{loc}$
- Laplace eq. → local field

⇒ Motion of surface atoms corrected; pulling effect of the field

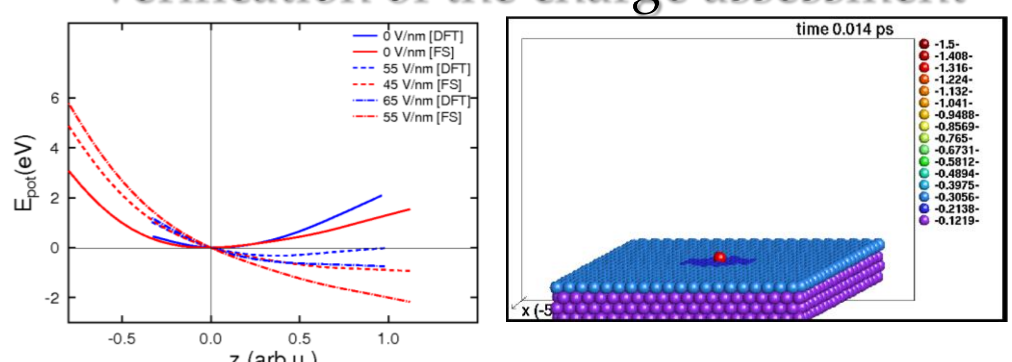
Laplace solution



- Model is submitted for publication in **PRE**

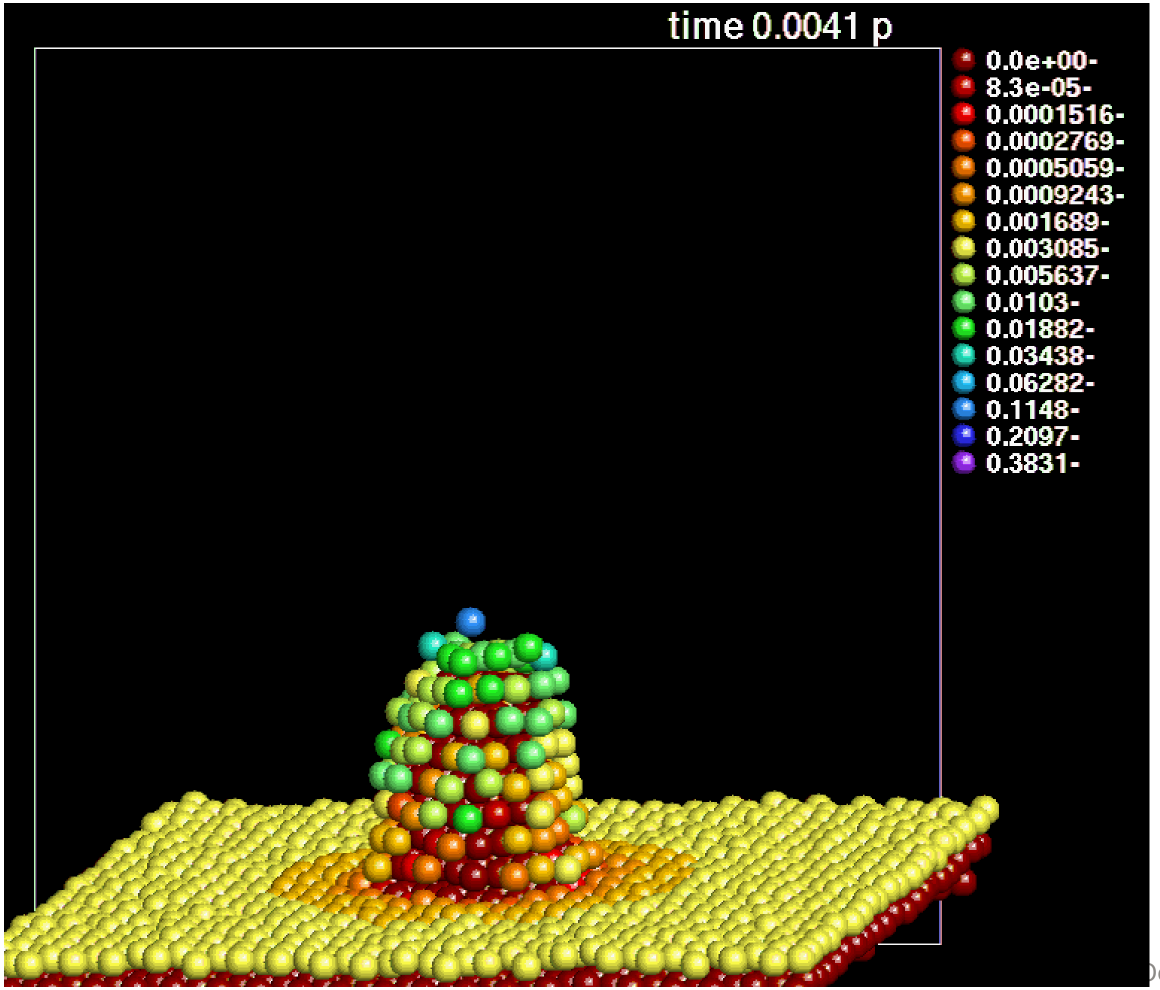
F. Djurabekova, S. Parviainen, A. Pohjonen, K. Nordlund, *"Atomistic modelling of metal surfaces under electric fields: direct coupling of electric fields to a molecular dynamics algorithm"*

Verification of the charge assessment



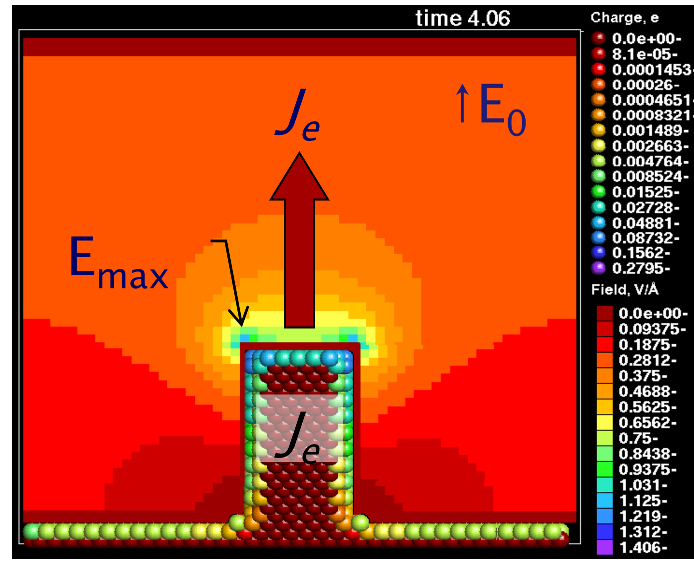
[DFT] results from T. Ono et al. Surf.Sci., 577,2005, 42

Short tip on Cu (100) surface at the electric field 10 V nm^{-1} (Temperature 500 K)

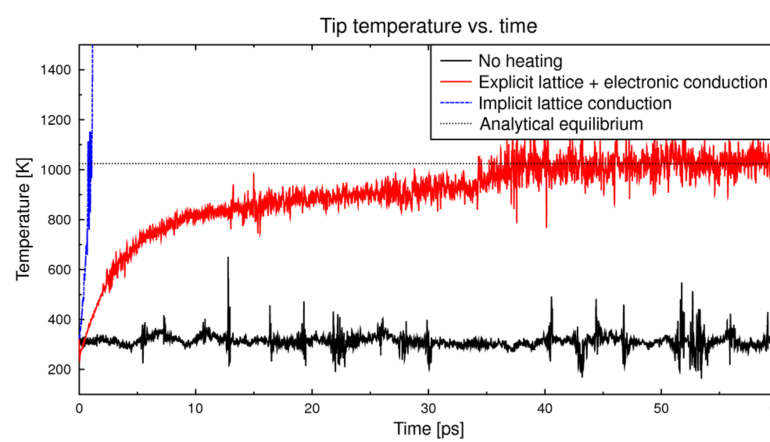


Stage 2: Dynamics of electrons for temperature account

- At such high electric fields, field emission is a non-negligible phenomenon
- Electrons escaping from the surface with significant current will heat the sharp features on the surface, causing eventually their melting.
- The change of temperature (kinetic energy) due to Joule heating and heat conduction is calculated by the 1D heat equation

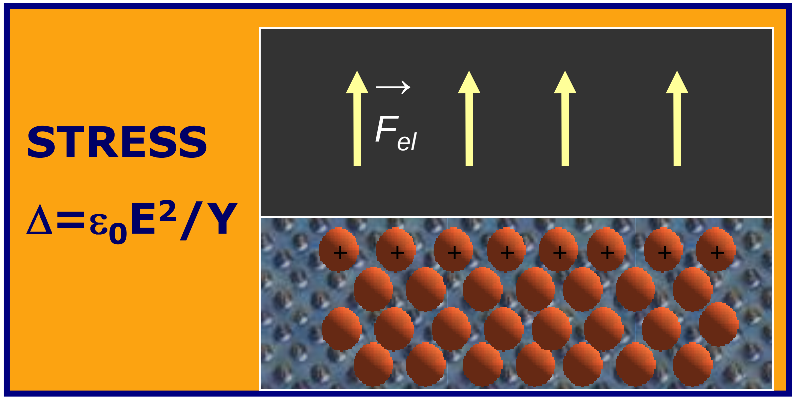


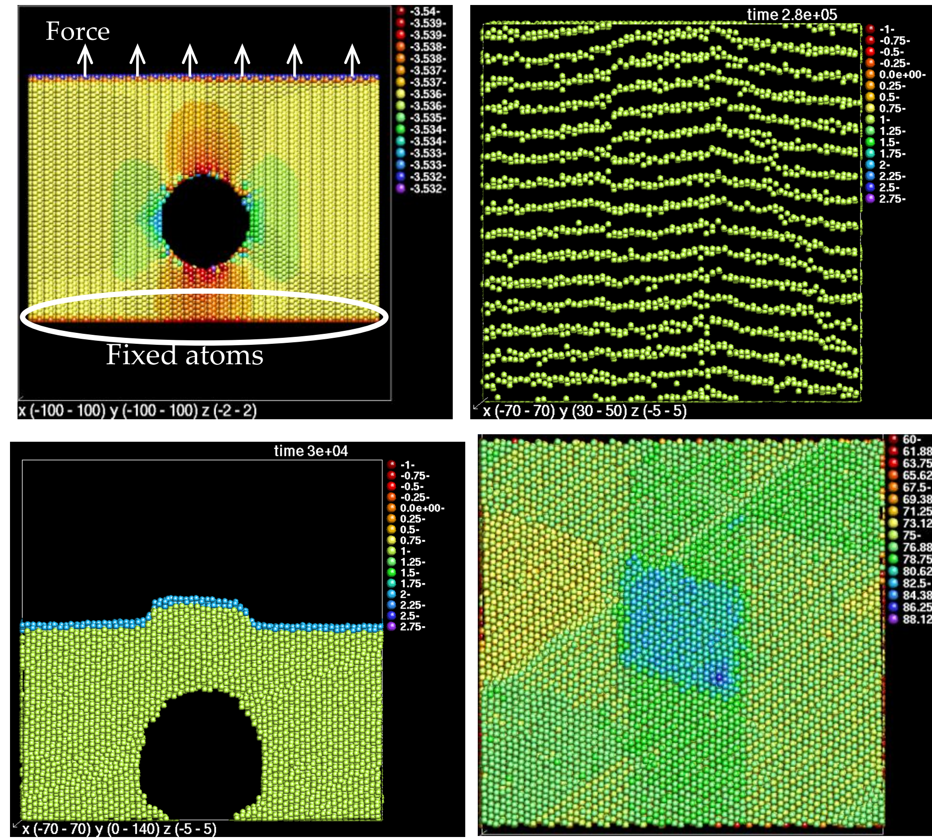
$$\frac{\partial T(x,t)}{\partial t} = \frac{K}{C_V}\frac{\partial^2 T(x,t)}{\partial x^2} + \frac{\rho(T(x,t))J^2}{C_V}$$



Results are submitted to **Comput. Mater. Sci.**,
S. Parviainen, F. Djurabekova, H. Timko, and K. Nordlund, *"Implementation of electronic processes into MD simulations of nanoscale metal tips under electric fields "*

Stage 3a: Onset of tip growth



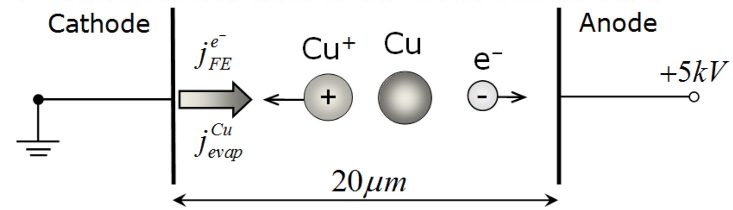


- Presence of an electric field exerts a tensile stress on the surface
- Presence of a near-to-surface void may trigger the growth of a protrusion

Submitted to **PRB: Rapid Commun.**,
A. S. Pohjonen, F. Djurabekova, A. Kuronen, and K. Nordlund, *"Dislocation nucleation from near surface void under static tensile stress in Cu"*

Stage 4: Plasma evolution

Corresponding to experiment...



1d3v electrostatic PIC-MCC code; included phenomena:

Start from these

- Cu evaporation, e- field emission (Fowler-Nordheim eq)

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

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

Create ions

- Collisions, esp. ionisation collisions

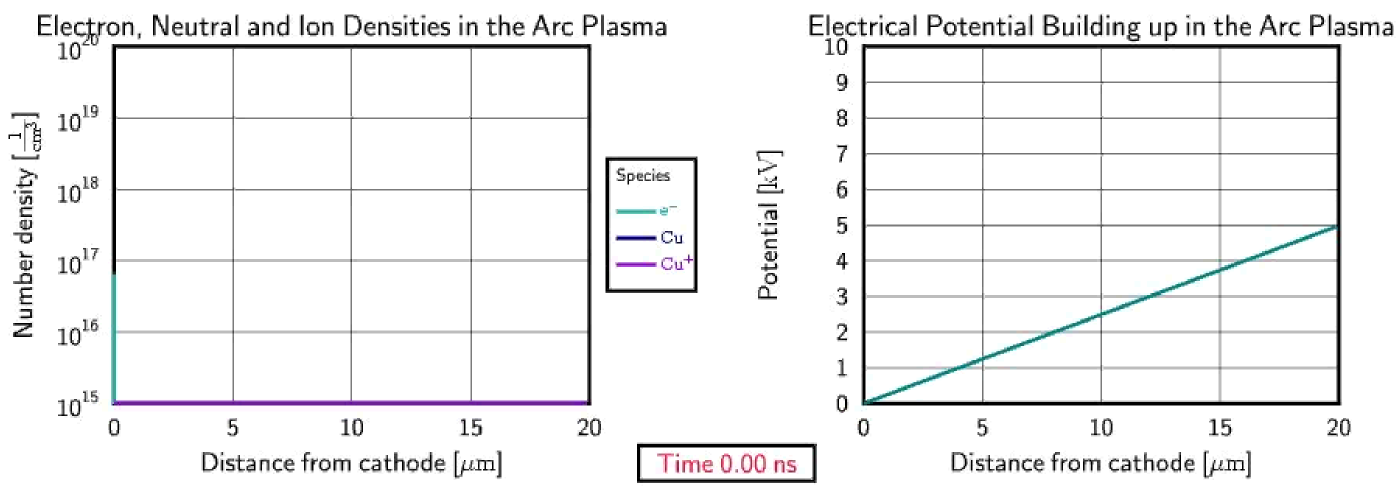
More e^- and Cu

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

Accepted for publication in **Contrib. Plasma Phys.**,
H. Timko, K. Matyash, R. Schneider, F. Djurabekova, K. Nordlund, A. Hansen, A. Descoeudres, J. Kovermann, A. Grudiev, W. Wuensch, S. Calatroni, and M. Taborelli ,
"A One-Dimensional Particle-in-Cell Model of Plasma Build-up in Vacuum Arcs"

Plasma build-up

- If not regulated externally, densities grow steadily
  - Only limiting factor: Energy available
- During onset, the plasma does not thermalize, is far from MB distribution (fluid approach not possible)



Under what conditions will an arc form?

Two conditions need to be fulfilled: (→ scaling btw. DC and RF)

- High enough **<u>initial local field</u>** to have growing FE current
- Reaching a **<u>critical neutral density</u>** → ionisation avalanche

- The sequence of events leading to plasma formation:

High electric field

Electron emission, neutral evaporation

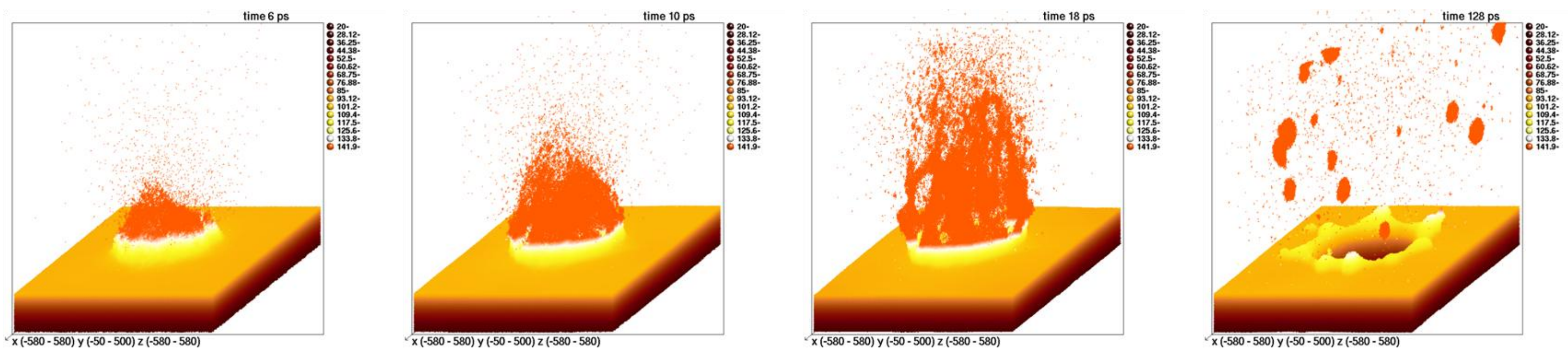
Ionisation ⇒ e^-, Cu and Cu^+ densities build up

Sputtering neutrals

- "Point of no return": $l_{mfp} < l_{sys}$ – corresponding to a critical neutral density ~ 10^{18} 1/cm^3 in our case ⇒ ionisation avalanche

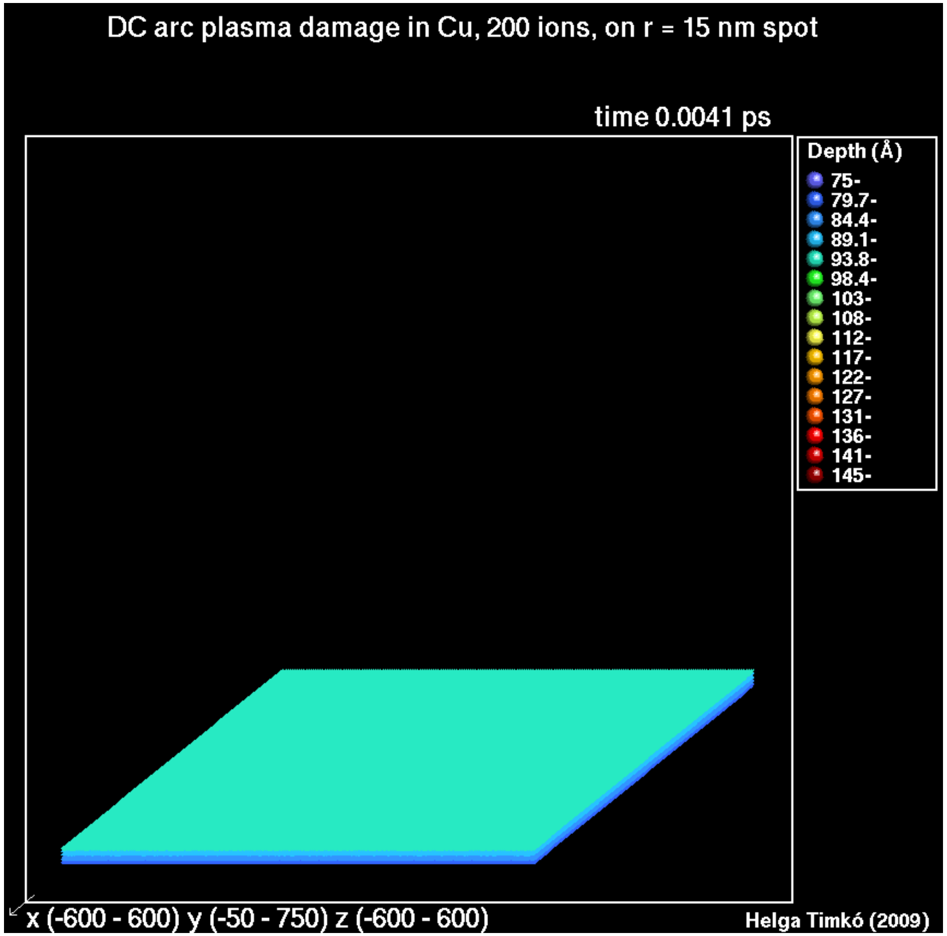
Stage 5: Cathode damage due to ion bombardment

- Knowing flux & energy distribution of incident ions, erosion and sputtering was simulated with MD
- Flux of ~10^{25} cm^{-2}s^{-1} on e.g. r=15 nm circle $\Rightarrow$ 1 ion/20 fs



H. Timko, F. Djurabekova, K. Nordlund, L. Costelle, K. Matyash, R. Schneider, A. Toerklep, G. Arnau-Izquierdo, A. Descoeudres, S. Calatroni, M. Taborelli , and W. Wuensch, "*Mechanism of surface modification in the plasma-surface interaction in electrical arcs*", **Phys. Rev. B 81**, 184109 (2010)

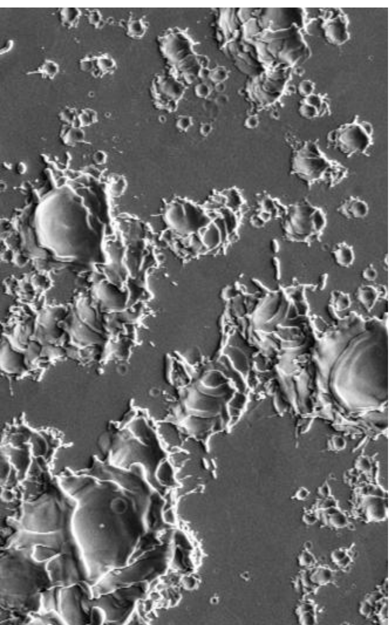
Mechanism of surface modification

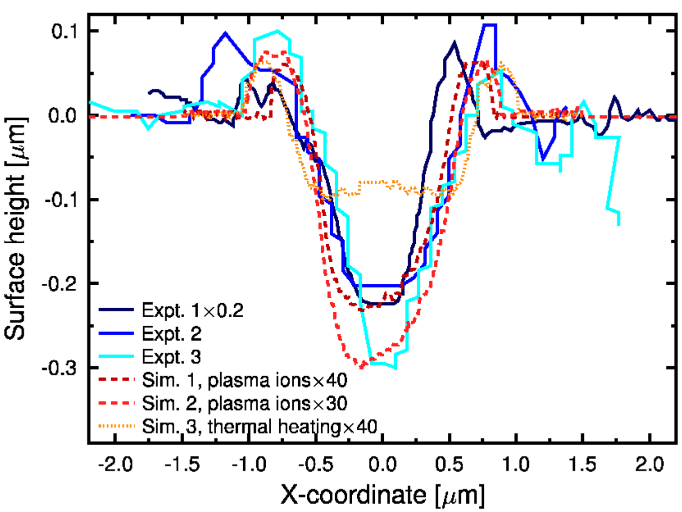


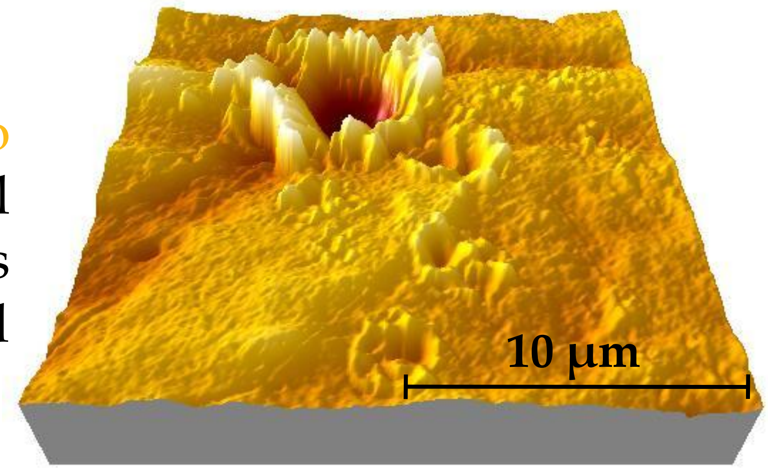
Comparison to experiment

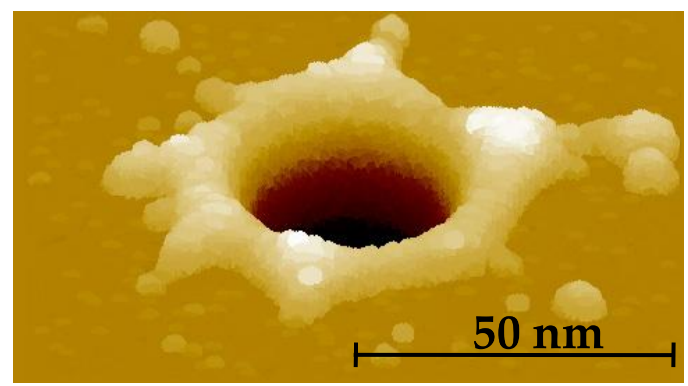
- Self-similarity:

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

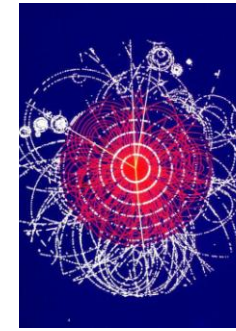




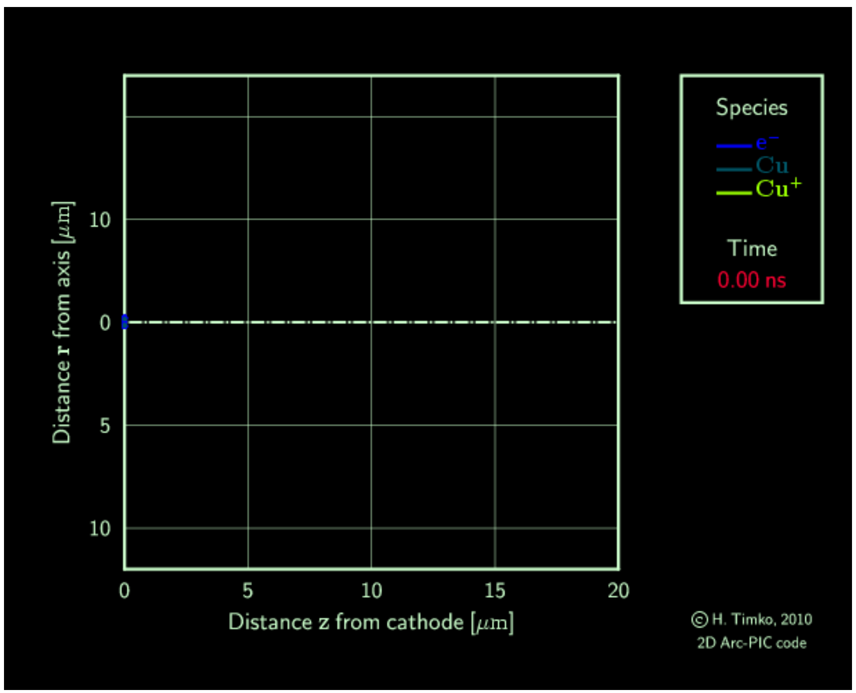




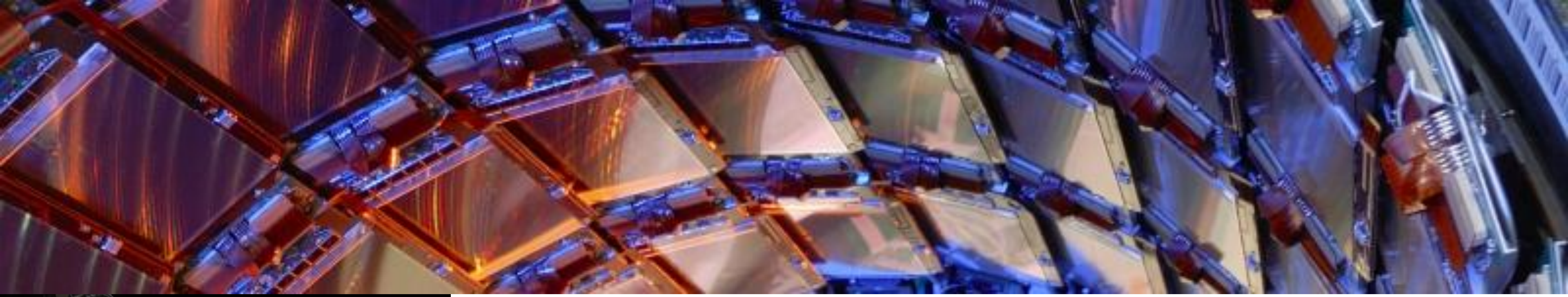
Summary and Outlook

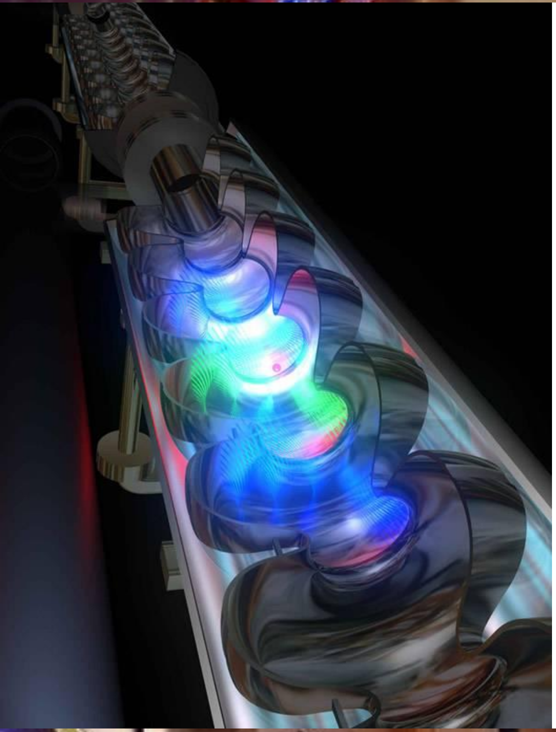


New 2D Arc-PIC code

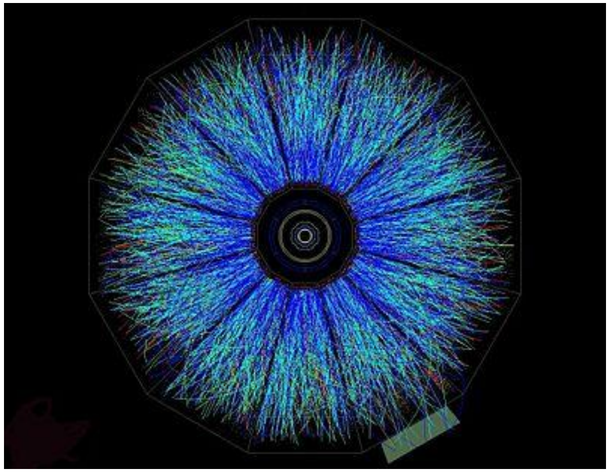


- We have established a ranking of materials and understood many bits and pieces of the puzzle already
- Still many open questions remain. To answer them, we need a close interaction between *theory and experiment*
  - Future of DC experiments: To test more basic physics
  - Multi-scale model: Give predictions to their outcome





Interested? Come to our Breakdown workshop *'MeVArc'* June 27-30th, 2011 in Helsinki!



Thank you!