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HIP

Understanding the breakdown: new prospects?

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Contents

- Multiscale model to approach the problem of electrical breakdown
- Surface charge, electronic effects
- Dislocations as a media of surface response to electric fields
- Electric discharges near a metal surface
- Summary and perspectives

Behind the model

University of Helsinki, Finland

Doc. Flyura Djurabekova
Senior scientist

Prof. Kai Nordlund

M Sc Aarne Pohjonen
Dislocations

M Sc Stefan Parviainen
Field emisssion and
neutral atom evaporation

M Sc Avaz Ruzibaev
Charges on surfaces

Dr Juha Samela
Sputtering and cratering

Dr. Helga Timko
Plasma simulations
(CERN, Switzerland)

Dr Lotta Mether
Plasma simulations
CERN, Switzerland

Inspiration comes from CERN, Geneva

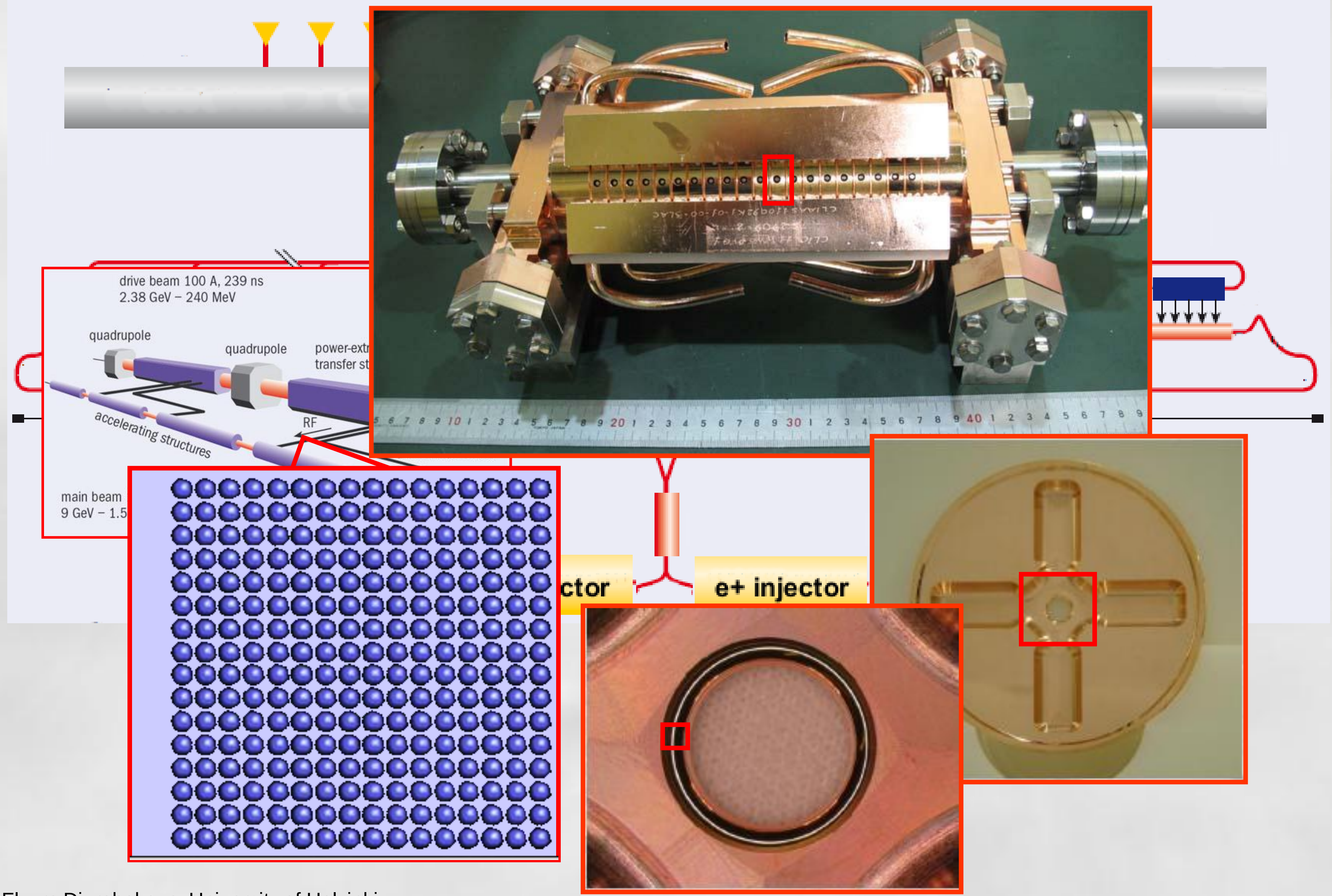
Dr. Walter Wuensch

Sergio Calatroni

Collaborators out of UH

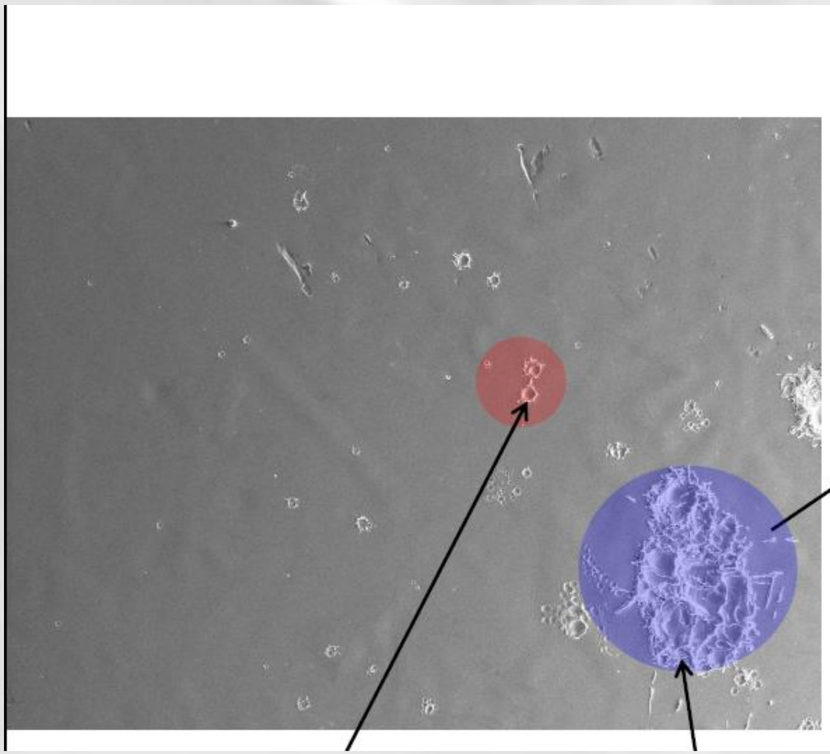
- **CERN**
  - Dr. Walter Wuensch – the main engine of the project
  - Sergio Calatroni – supervision of dc experiments
  - PhD students, involved in the same experiments
  - Dr. Tomoko Muranaka – field emission measurements+SEM imaging
  - Dr. Markus Aicheler – mechanical properties of Cu surfaces
  - Dr.Helga Timko, Dr. Lotta Mether and MSc Kyrre Ness Sjoebaek – plasma simulations of onset of vacuum arc
  - Many-many others, who question and approve, criticize and support our modeling efforts!
- **Aalto university** (recently begun)
  - Prof. Filip Tuomisto – positron annihilation measurements
  - Prof. Roman Novak – nanoindentation measurements of Cu surface
- **Hebrew University of Jerusalem**
  - Dr. Yinon Ashkenazy – atomistic simulations of dislocations in nanostuructures
- **Tartu University, Estonia**
  - Dr. Vahur Zadin – FEM calculations of real surfaces
  - PhD studetns

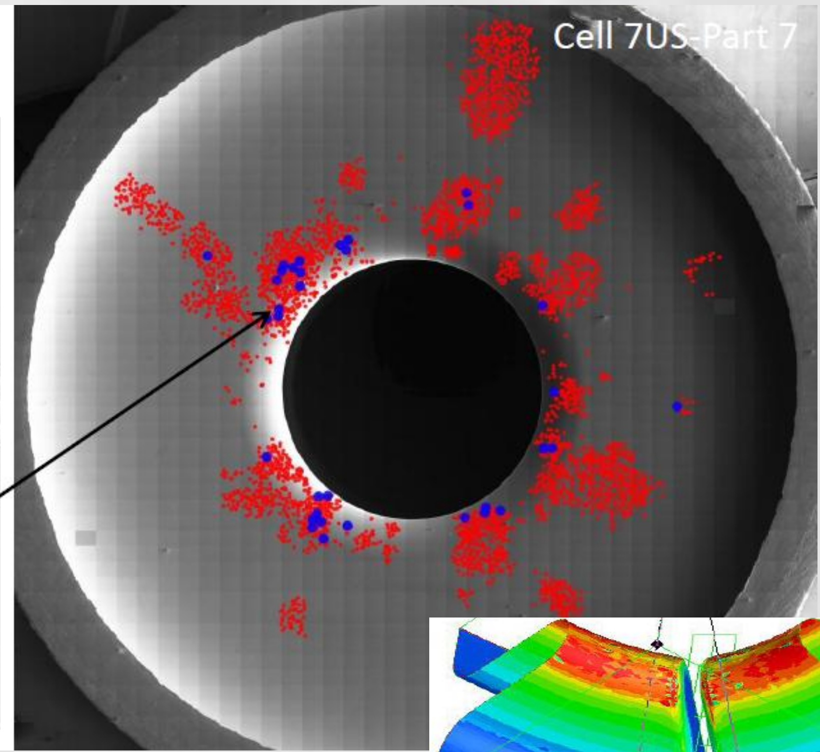
CLIC: "Compact" Linear Collider…

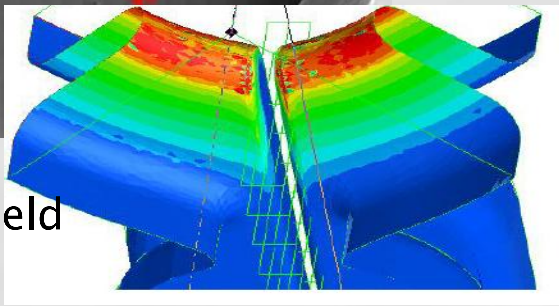


Problem: no metal withstands nominal accelerating gradients (~150 MV/m)

- Interactions of high gradient electromagnetic fields result in frequent breakdown events





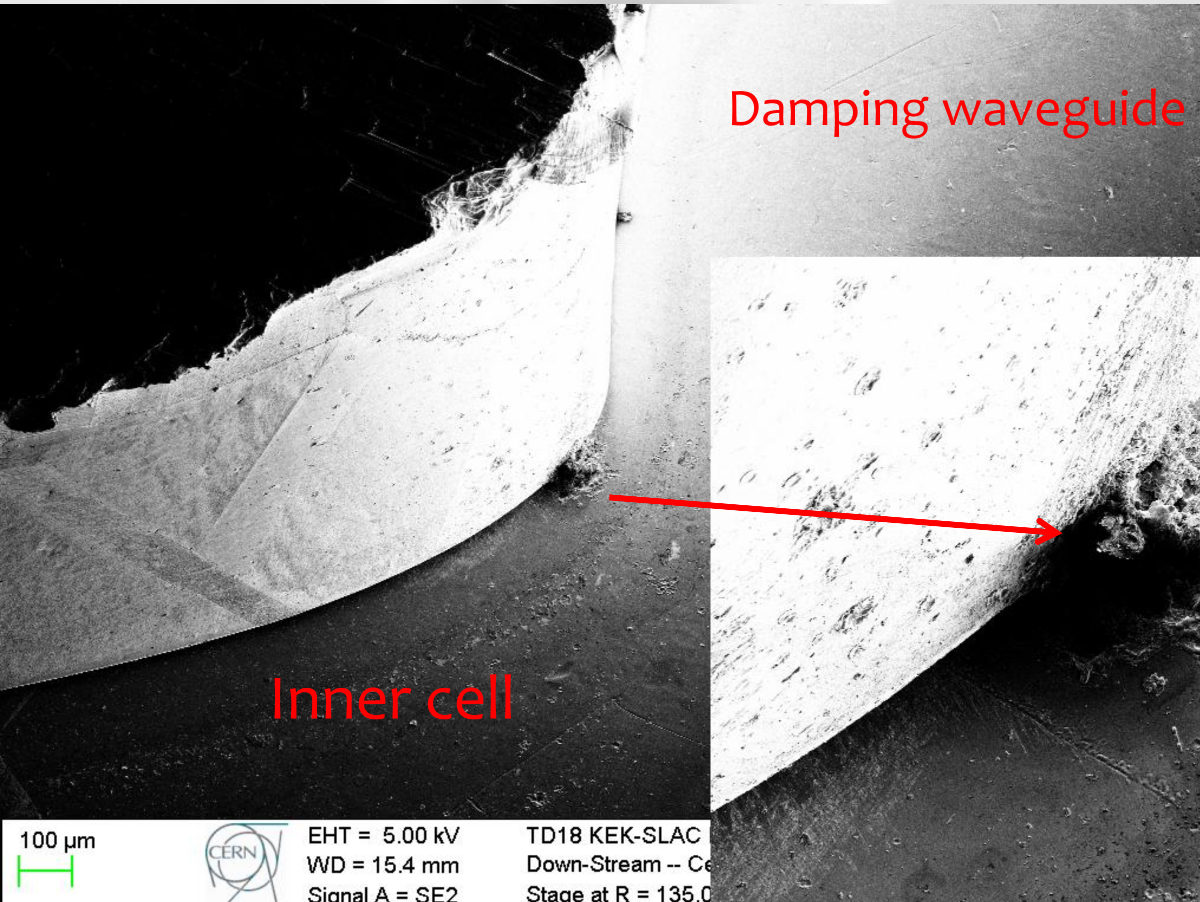


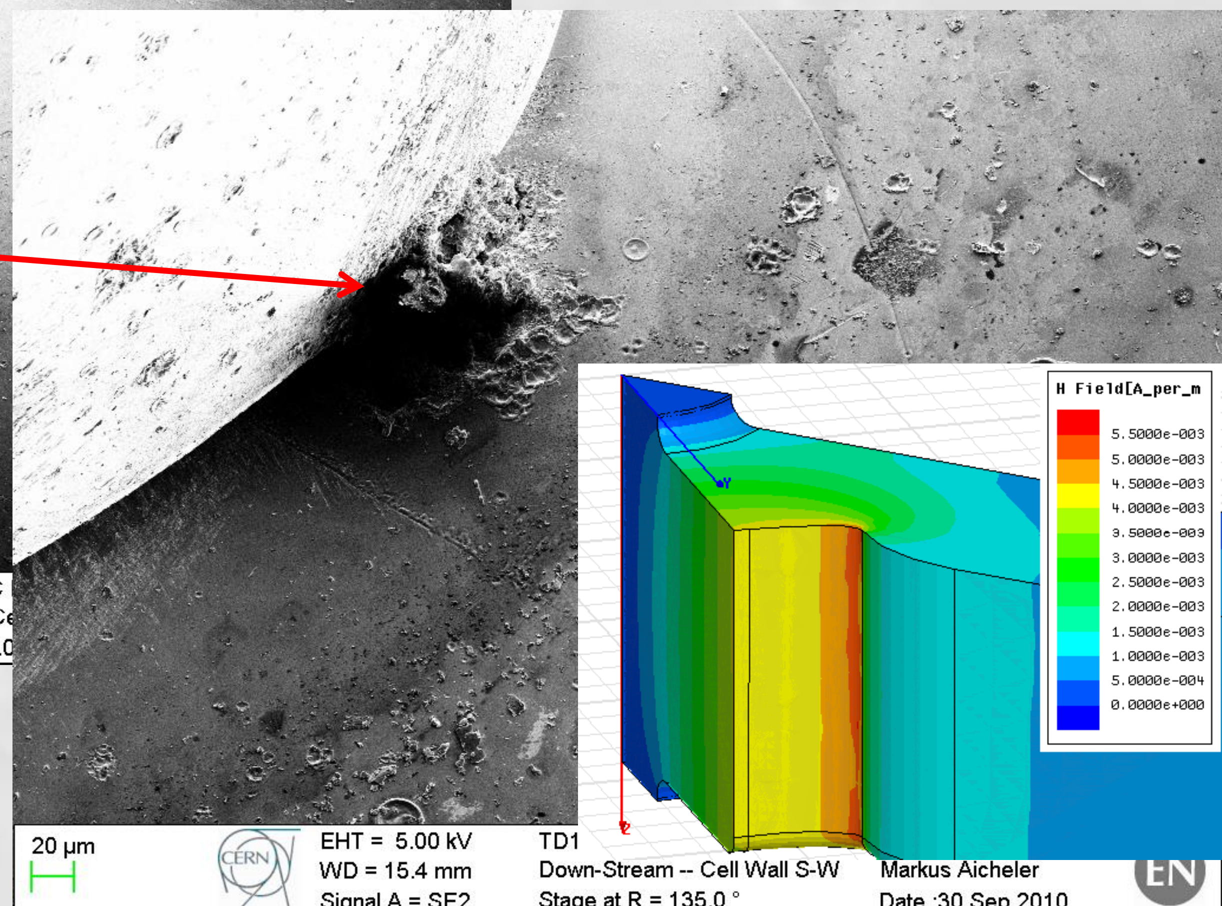
Courtesy of M. Aicheler, CERN

Macroscopic electromagnetic field near irises

High currents destroy the high precision shapes

Current density around $2\times10^{8} A/cm^{2}$ during test





Courtesy of W.Wuensch, CERN

Test performance of sophisticated Cu structures

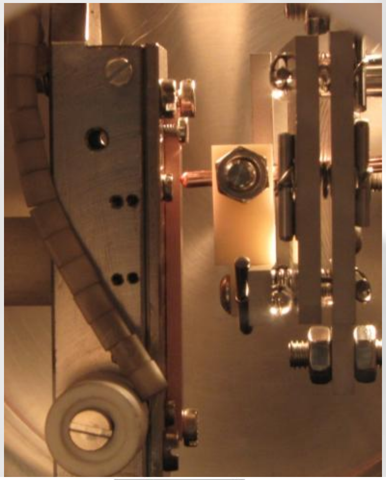
- The surface imperfection alone cannot explain all the nature of breakdown phenomenon.
- Japanese group at KEK consistently tested differently prepared Cu surfaces.
- They saw that only internal impurities , and structural defects may explain a similar behavior.

Results of High Gradient Tests

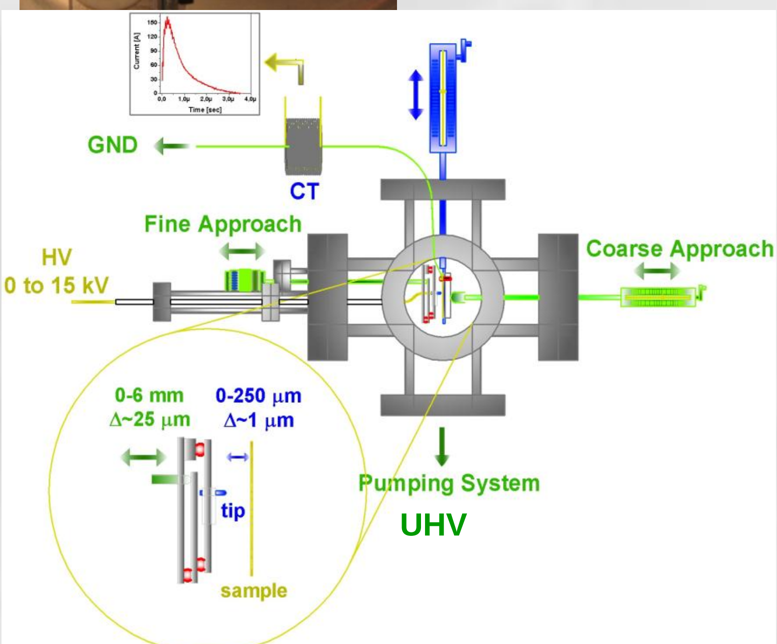
- Sophisticated fabrication technologies for X-band high gradient accelerating structures successfully developed at KEK with SLAC, INFN and CERN.
- We compared breakdown rate for three A3.75-T2.6 copper structures, one OFC copper, 6N copper treated with HIP, and 7N large grain copper. But rf breakdown performance was almost same.
- The nearly perfect surface processing affected only processing time. Ultra-clean structures conditioned faster then the normally processed structure.

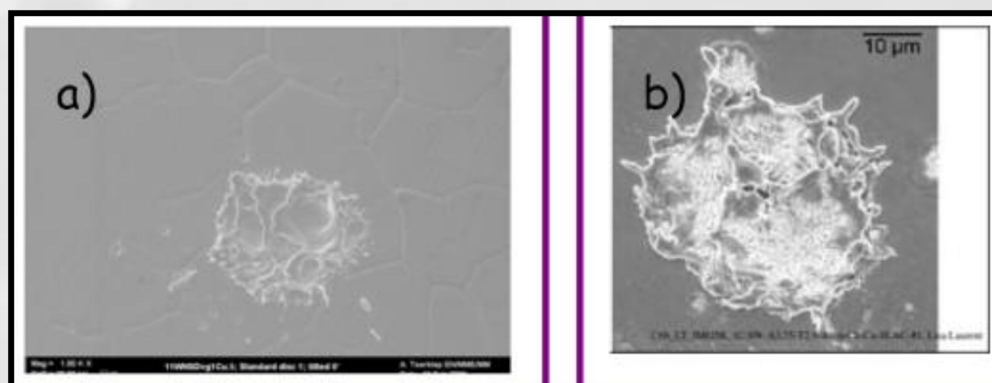
Courtesy of Y. Higashi, KEK, Japan after MeVARC-3

Rf-breakdowns and dc-sparks

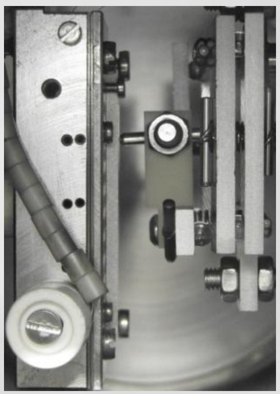


- To investigate the sparking in rf accelerating structures, the simplified dc-spark testing station has been set up in CERN
  - Inspecting closely the surface damage spots left by small sparks of self-built plasma in vacuum, there is a clear self-similarity.
  - Although the nature of the damage in rf-experiments overall looks more complex, the experiments on dc sparks due to more simplified construction can help to understand the main driving forces behind the process of surface response on electric field effect

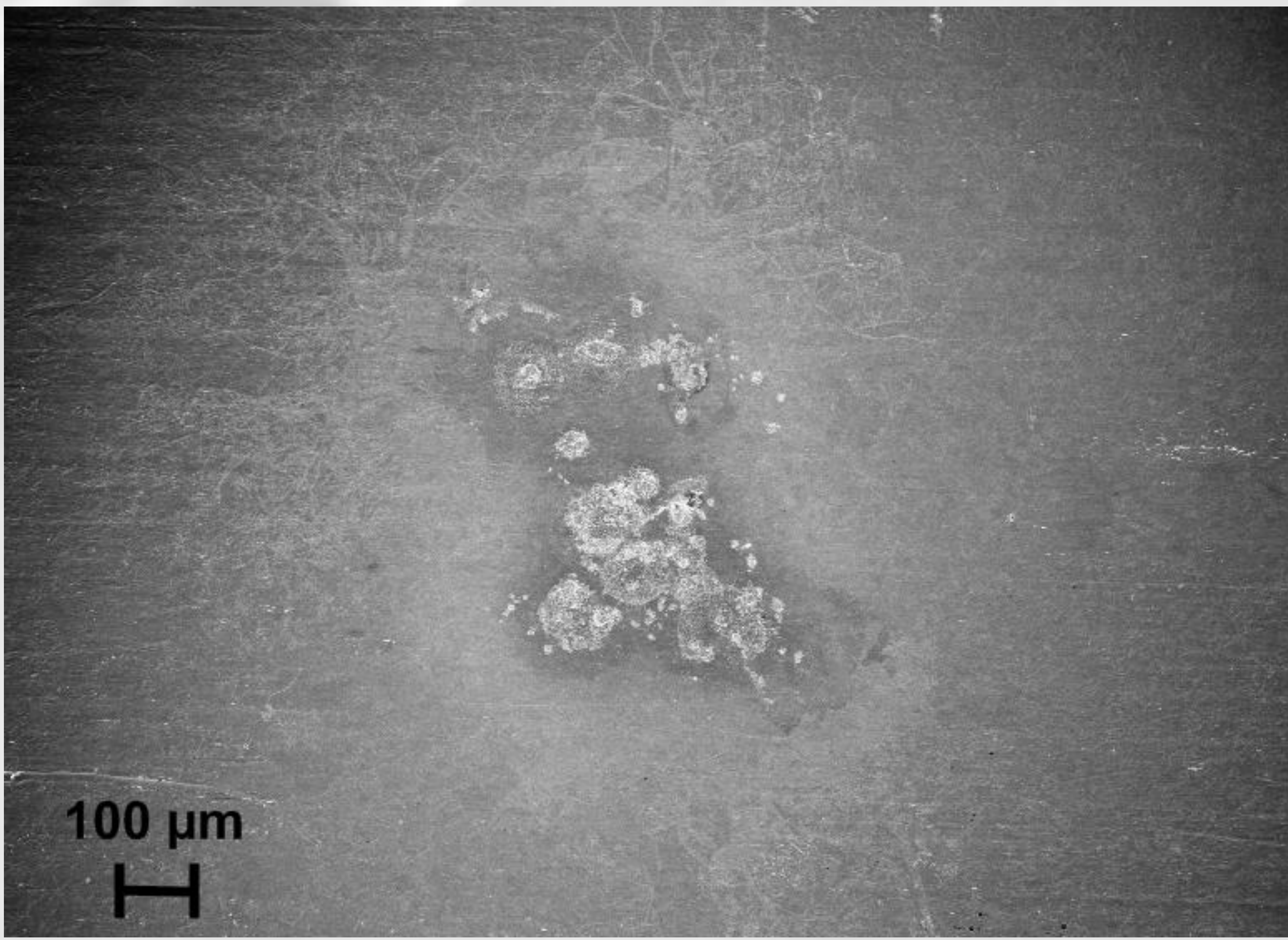




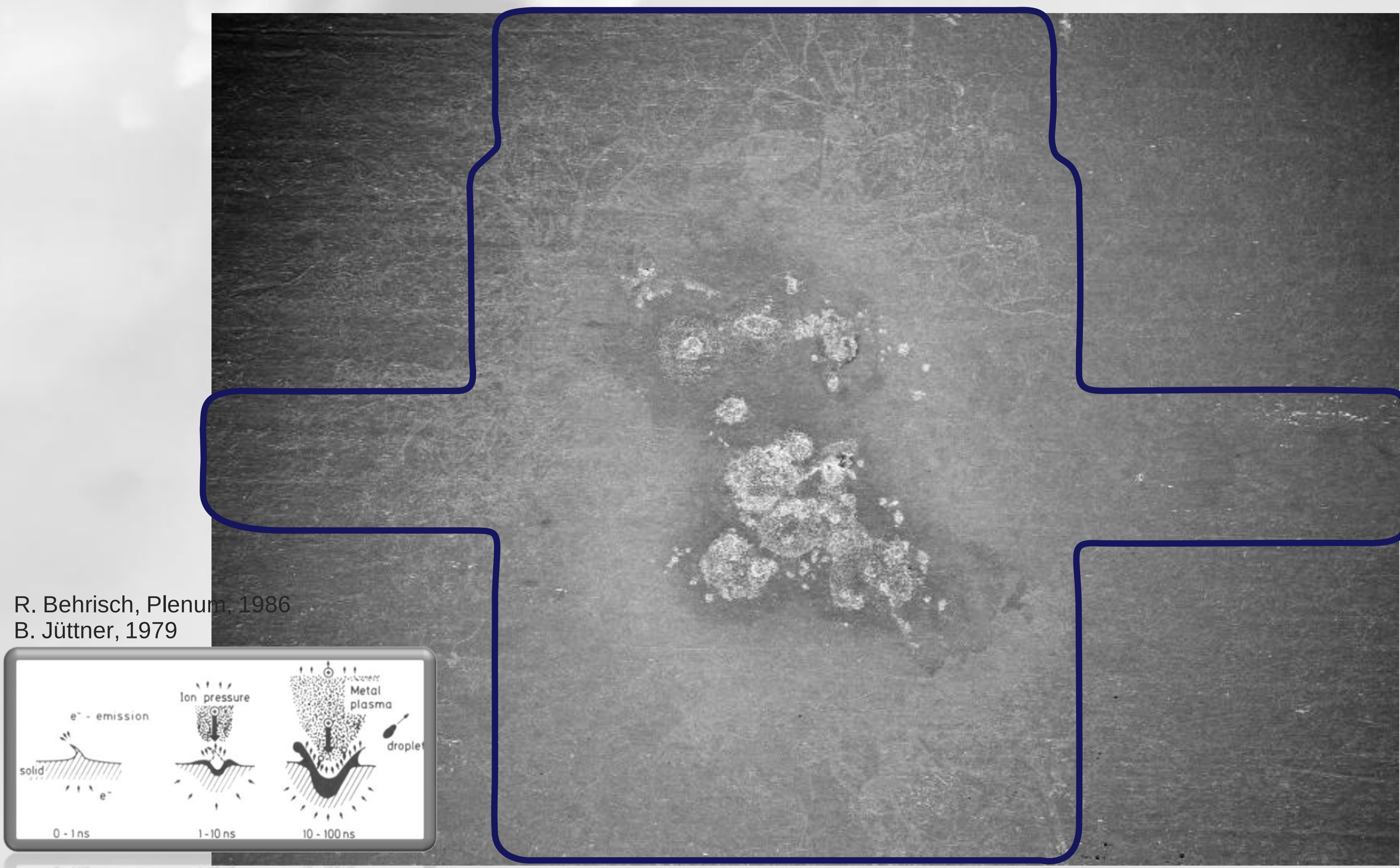
Problem at hand



Setup to measure dc sparks on a flat cathode surface (CERN)

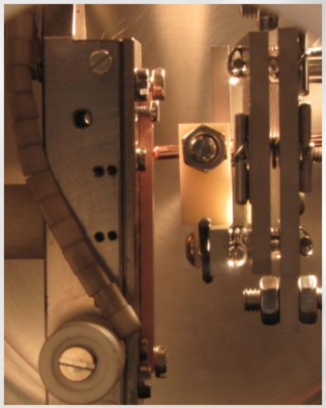


What to do?
Shape a model!



R. Behrisch, Plenum, 1986
B. Jüttner, 1979

…Multiscale/multiphysics computational model to simulate electrical breakdown



Stage 1: Charge distribution @ surface
Method: DFT with external electric field

~few fs

Stage 2: Atomic motion & evaporation
+
Joule heating (electron dynamics)
Method: Hybrid ED&MD model (includes Laplace and heat equation solutions)

~few ns

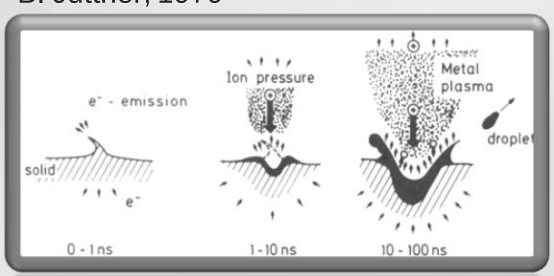
~ sec/min

~ sec/hours

Stage 3a: Onset of tip growth; Dislocation mechanism
Method: MD, ED+MD, FEM…

Stage 3b: Evolution of surface morphology due to the given charge distribution
Method: Kinetic Monte Carlo

R. Behrisch, Plenum, 1986
B. Jüttner, 1979



Stage 4: Plasma evolution, burning of arc
Method: Particle-in-Cell (PIC)

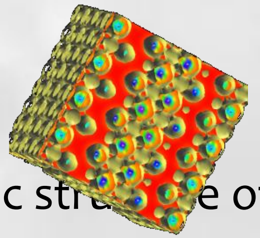
~10s ns

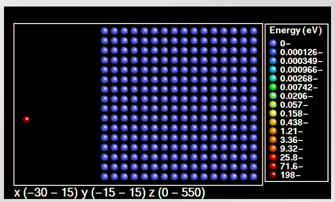
Stage 5: Surface damage due to the intense ion bombardment from plasma
Method: Arc MD

~100s ns

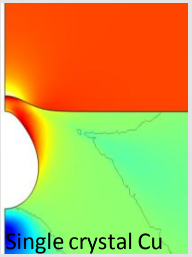
What tools we use:

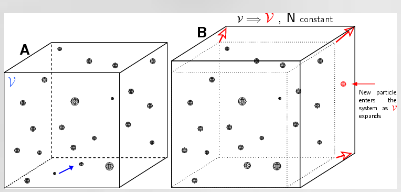
- In our group we use all main atomic-level simulation methods:
  - Density functional theory (DFT)
    - Solving Schrödinger equation to get electronic str[illegible]e of atomic system



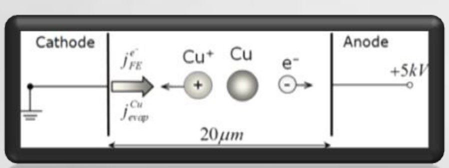


  - Molecular dynamics (MD)
    - Simulation of atom motion, classically and by DFT
  - Finite element method (FEM) COMSOL to mimic the macroscopic properties of surfaces



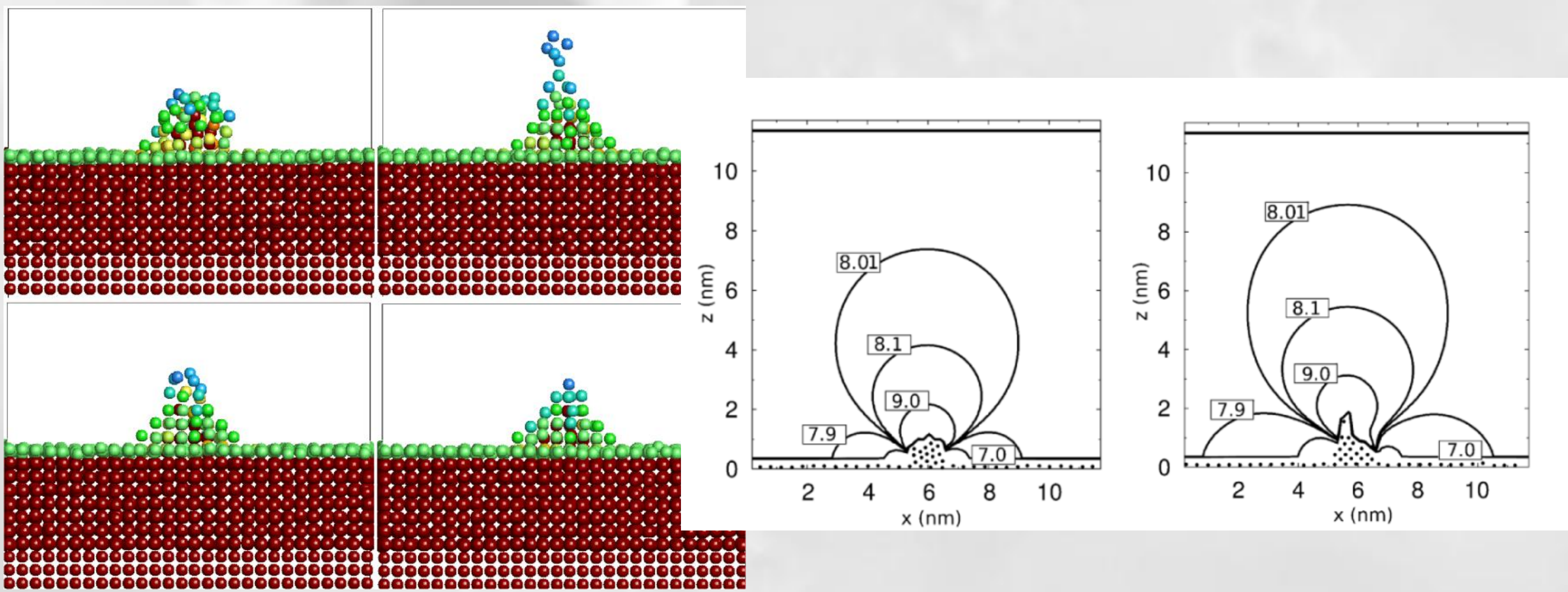


  - Kinetic Monte Carlo (KMC)
    - Simulation of atom or defect migration in time
  - Simulations of plasma-wall interactions
    - Simulation of plasma-particle interactions with surfaces



- We use all of them to tackle the arcing effects!

Where to start?
Electrodynamics–molecular dynamic model

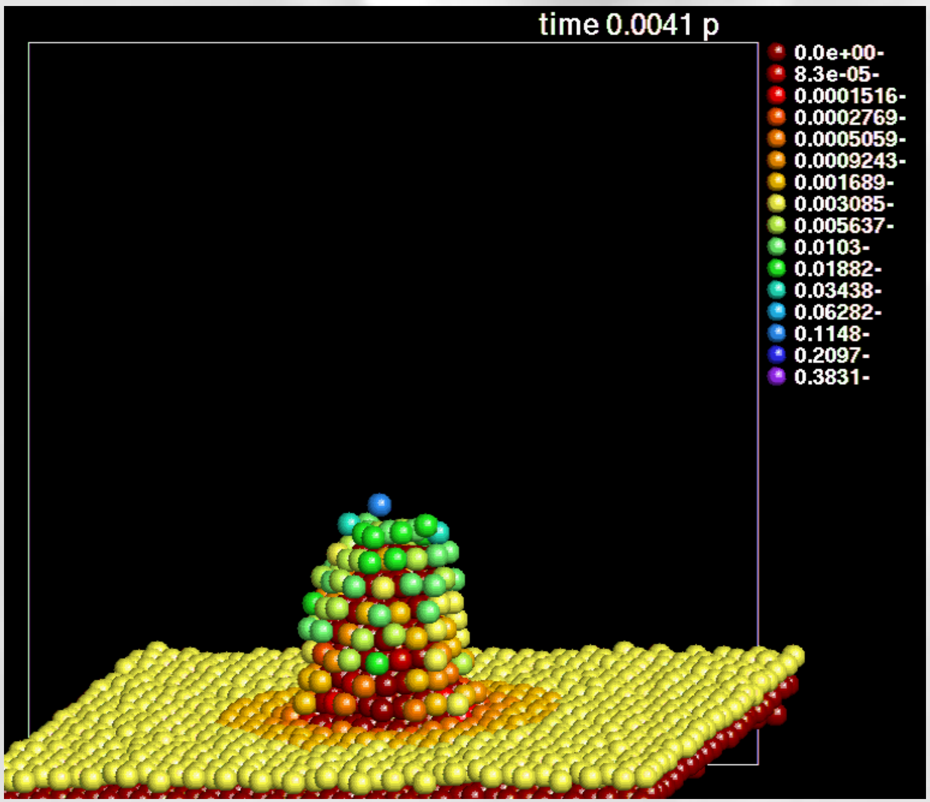


Details in F. Djurabekova, S. Parviainen, A. Pohjonen and K. Nordlund, Phys. Rev. E 83, 026704 (2011).

- ED-MD model follows the evolution of the charged surface.
- The dynamics of atom charges follows the shape of electric field distortion on tips on the surface

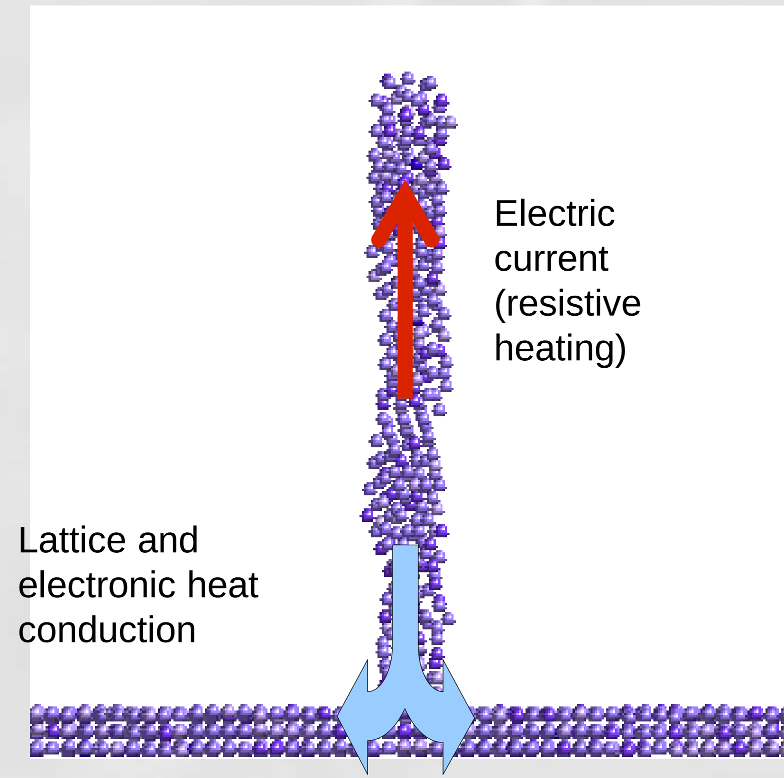
Effects of electric fields implemented in model

- At the field 1 GV/m and temperature 500K we managed to simulate the field assisted evaporation of atoms



Details in F. Djurabekova, S. Parviainen, A. Pohjonen and K. Nordlund, Phys. Rev. E 83, 026704 (2011).

- We also have a Joule heating of tips by field emission currents by solving 1D heat equation



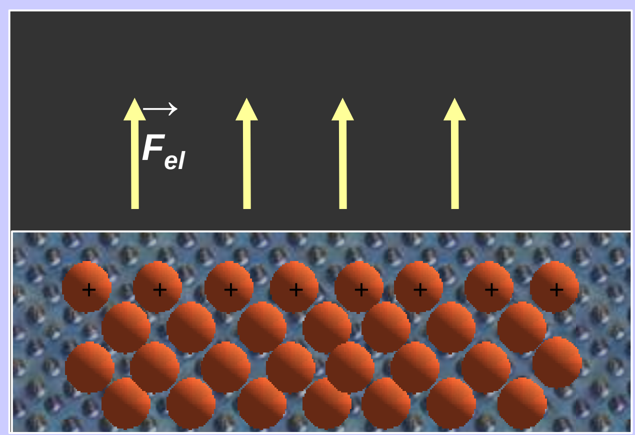
S. Parviainen, F. Djurabekova, H. Timko, and K. Nordlund, *Comput. Mater. Sci.* 50, 2075 (2011).

Onset of tip growth
Stresses due to the field

- Experimentally it was clearly observed that field emission starts from localized spots – field emitters (tips)
- But how would the tips be formed in the first place?
- While making the simulation of the atomic motion under an electric field (high values) we notice the significant expansion of the surface.
- This observation led us to think on the effect of the stress.

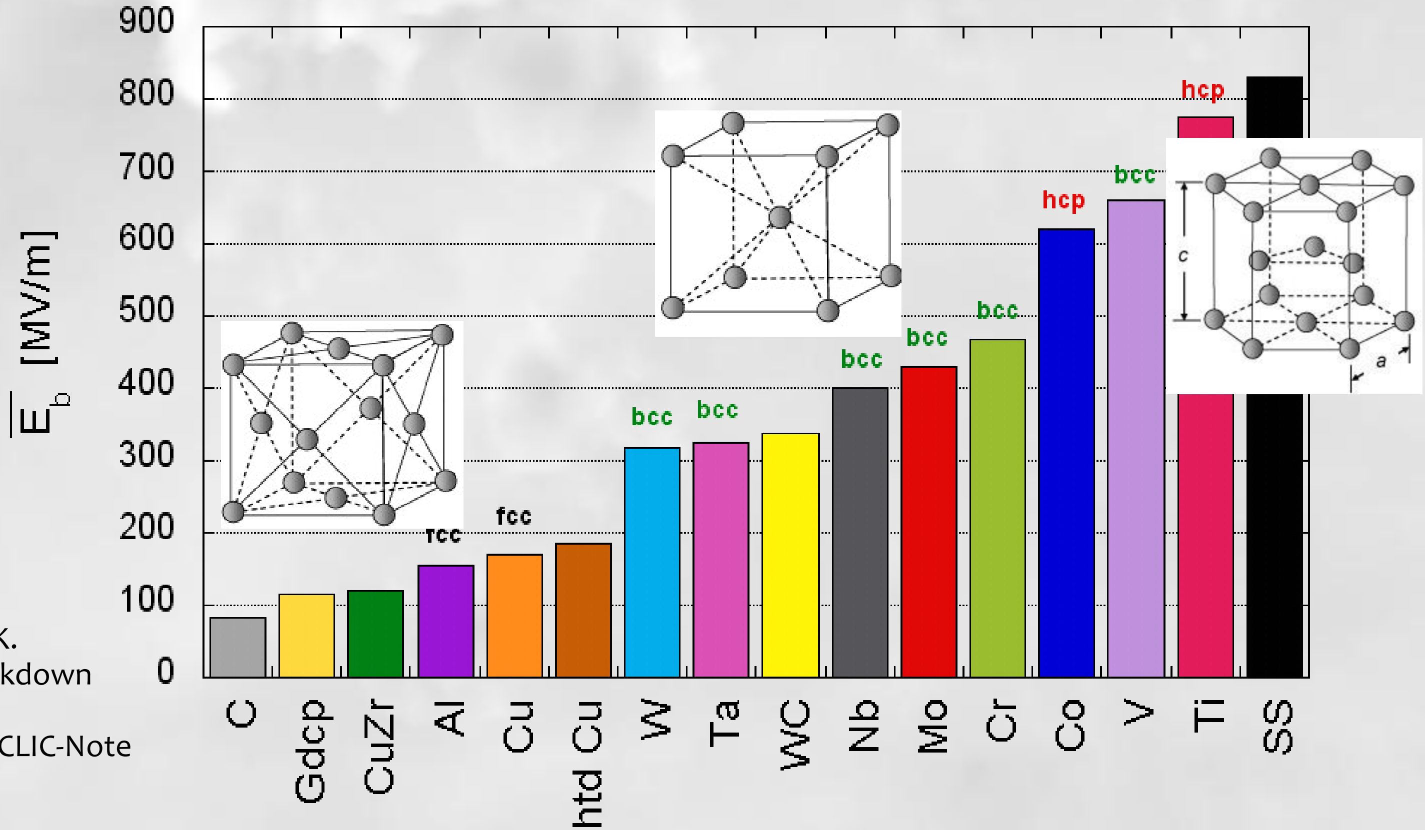
STRESS

$\Delta = \frac{1}{2}\varepsilon_0 E^2 / Y$



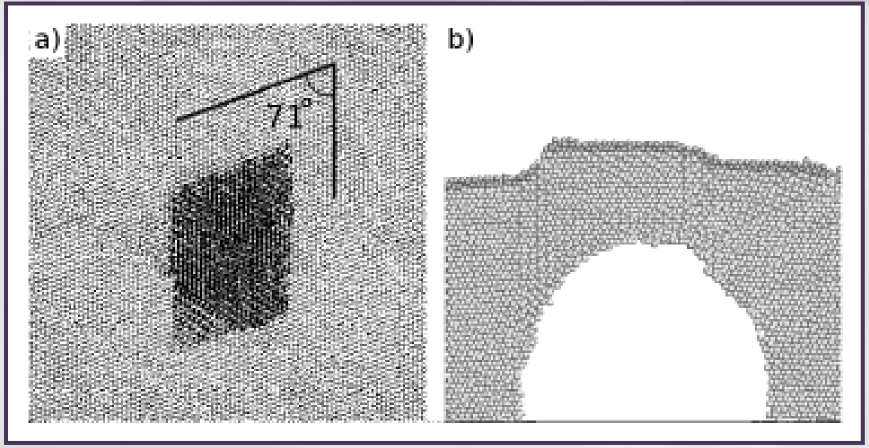
Correlation with crystal structure

- Experiments on the critical field for electric breakdown very well correlate with the crystal structure
  - Suggestive of a dislocation origin of the tip growth

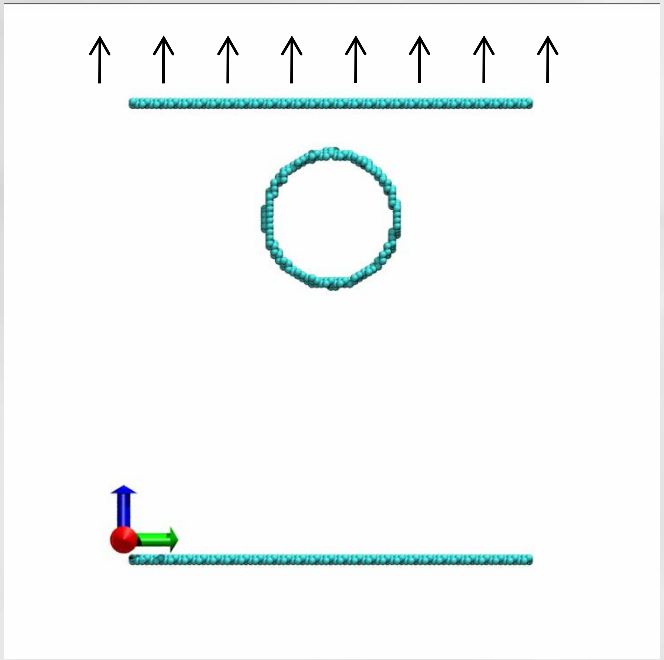


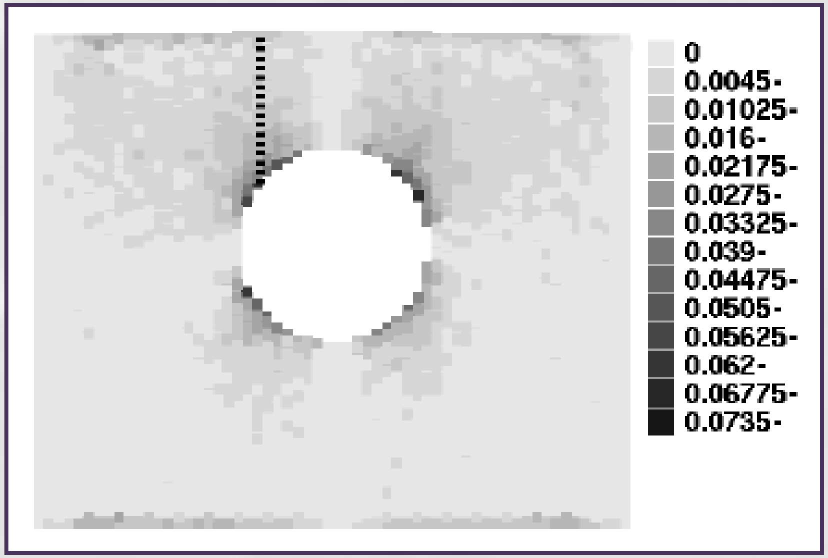
A. Descoeudres, F. Djurabekova, and K. Nordlund, DC Breakdown experiments with cobalt electrodes, CLIC-Note 875, 1 (2010).

Voids: the easy way to simulate a lattice distortion by MD



- We simulated a void near {110} Cu surface , when the high tensile stress is applied on the surface. Bottom is fixed, lateral boundary allowed to move in z direction.

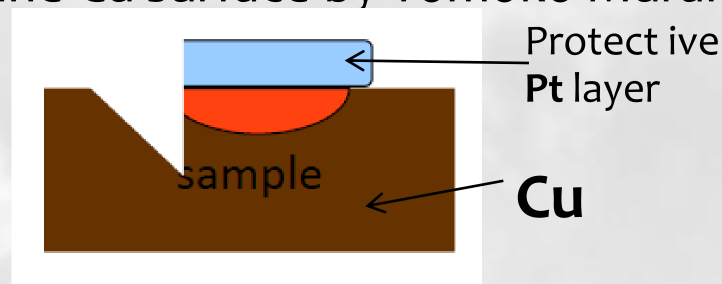


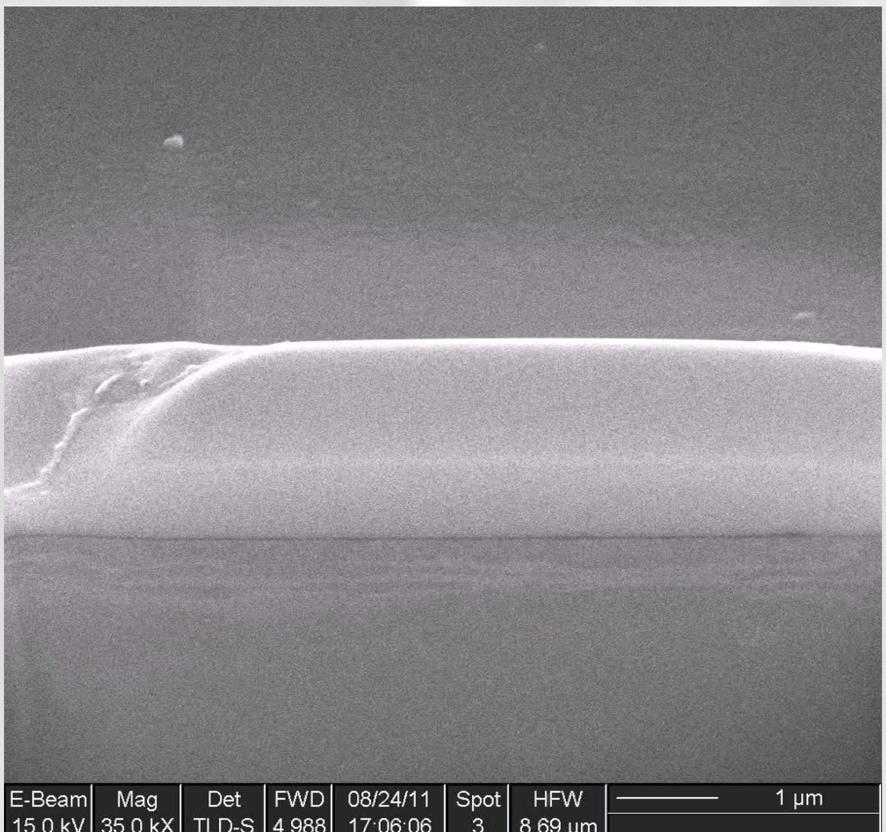


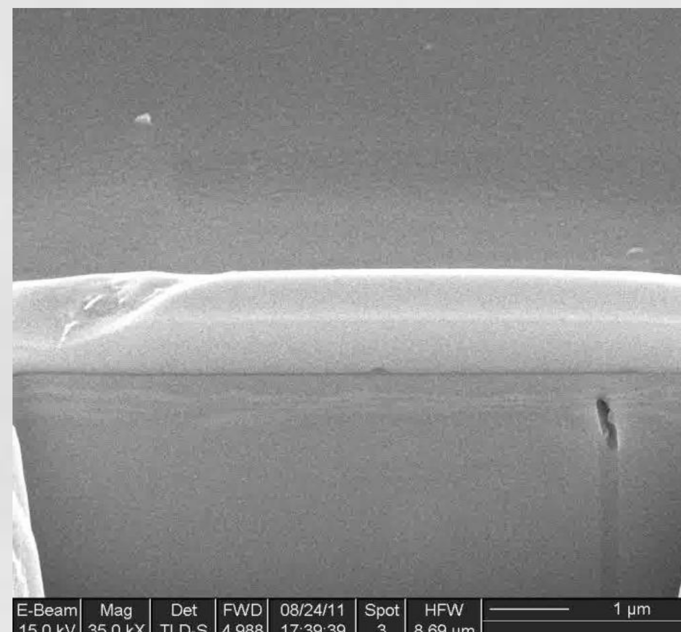
A. Pohjonen, F. Djurabekova, et al., Dislocation nucleation from near surface void under static tensile stress on surface in Cu, *Jour. Appl. Phys.* 110, 023509 (2011).

Are the voids real?

- SEM imaging combined with FIB helped to see a void at a random position in pristine Cu surface by Tomoko Muranaka (Uppsala Univ.)

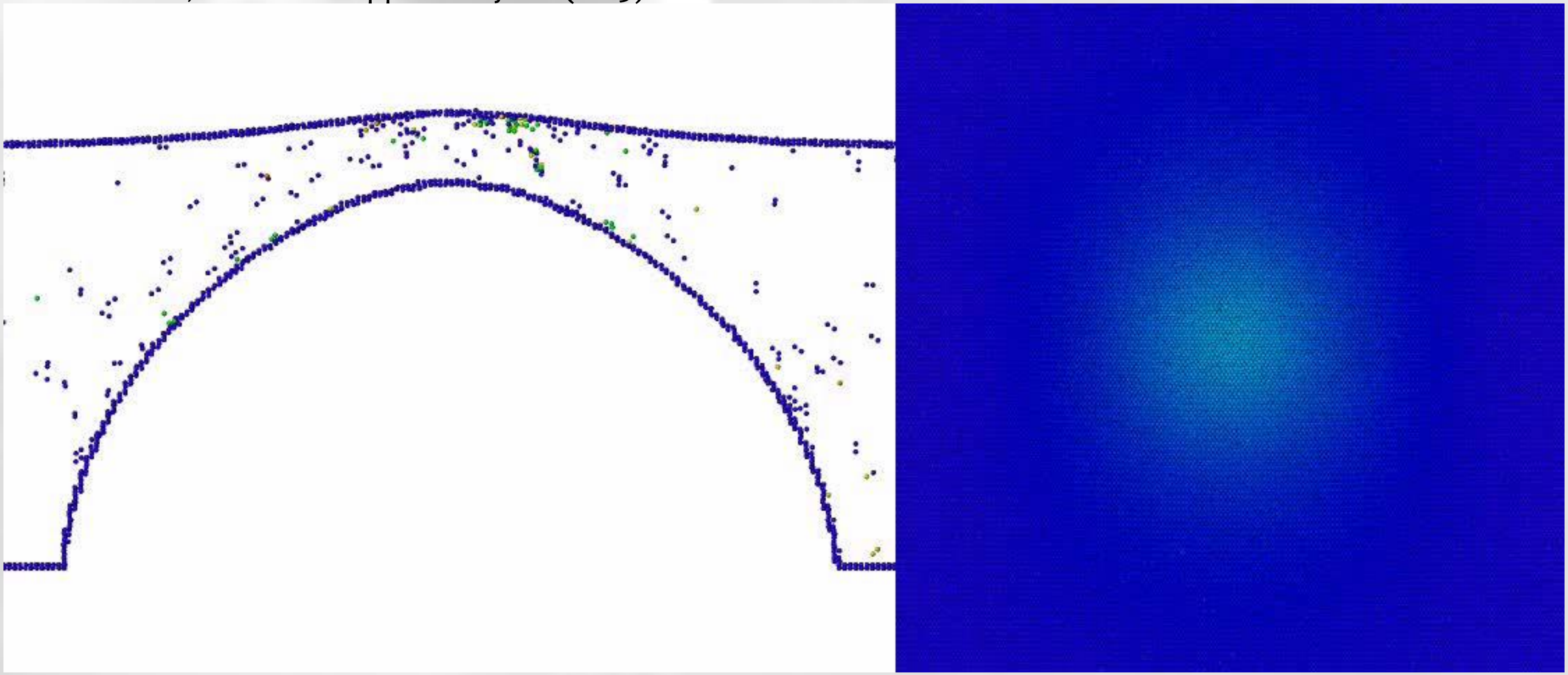






Combined ED–MD simulation of the surface with a void

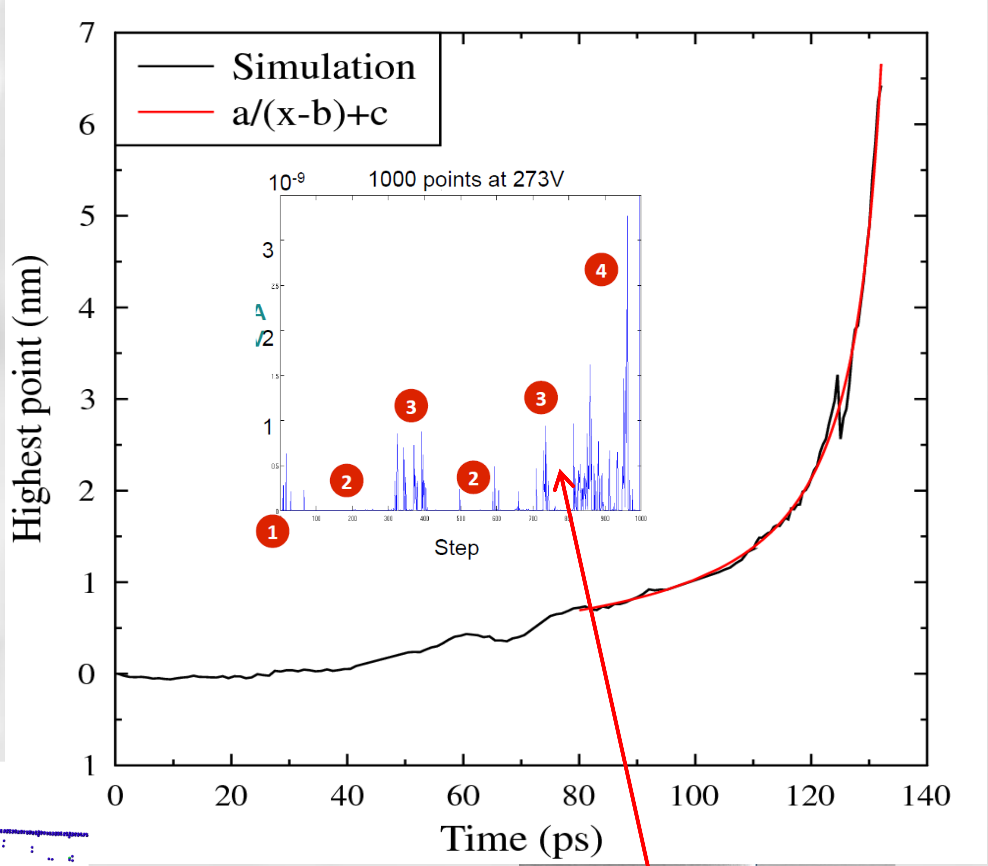
A. S. Pohjonen, S. Parviainen, T. Muranaka, and F. Djurabekova, Dislocation nucleation on a near surface void leading to surface protrusion growth under an external electric field, Journal of Applied Physics (2013).

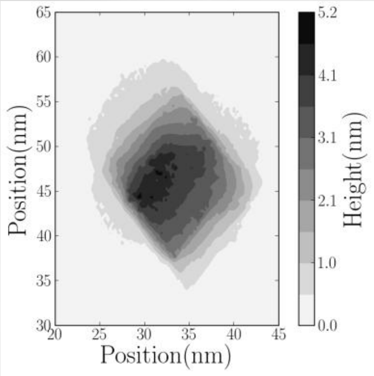


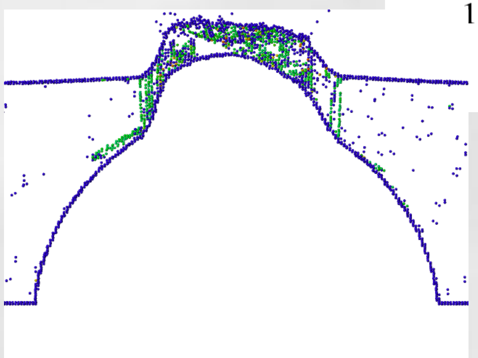
- We have now finished the analysis of the behavior of a void under tensile stress due to the electric field (Simulations now done with the hybrid ED–MD code, where the electric field effect is accounted explicitly)

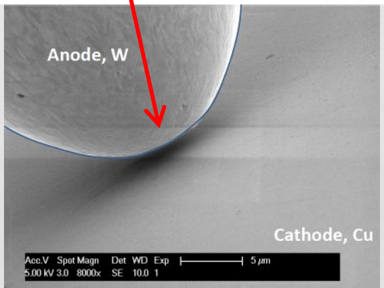
The gradual growth seen with unilateral tensile stress on surface is “catastrophic” in the presence of the field

- The analysis of the protrusion height increase shows an asymptotic character. Once it starts growing, the self-reinforcing effect of the field enhancement around the tip of the protrusion causes the increase of its height in the ”catastrophic” manner









Dislocation-based model for electric field dependence

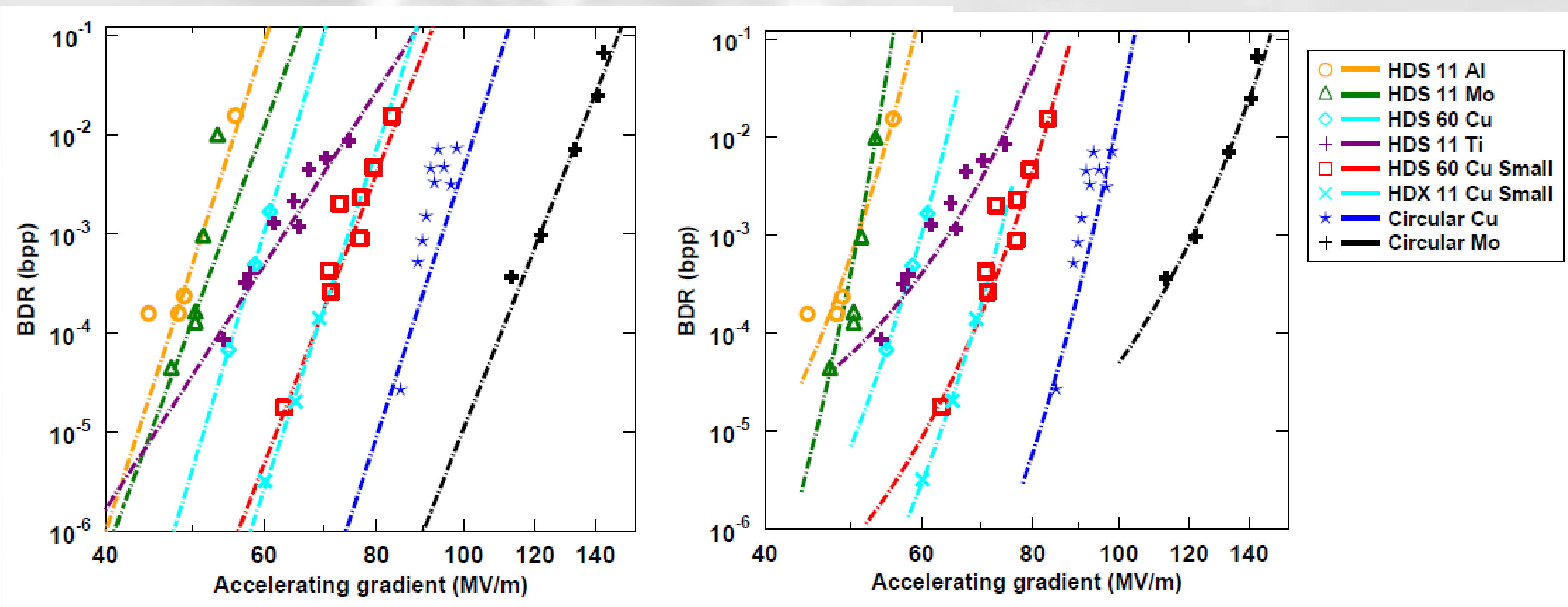
- Now to test the relevance of this, we fit the experimental data
- The result is:

$$BDR = AE^{29}$$

Power law fit

$$BDR = Ae^{\varepsilon_0 E^2 \Delta V / kT}$$

Stress model fit



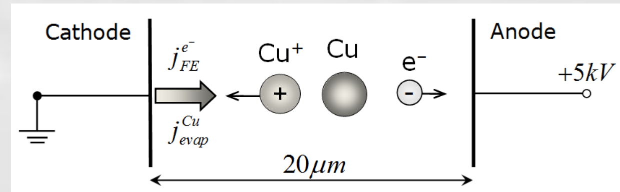
[W. Wuensch, public presentation at the CTF3, available online at http://indico.cern.ch/conferenceDisplay.py?confId=8831. with the model.]

[K. Nordlund and F. Djurabekova, Defect model for the dependence of breakdown rate on external electric fields, Phys. Rev. ST-AB 15, 071002 (2012)]

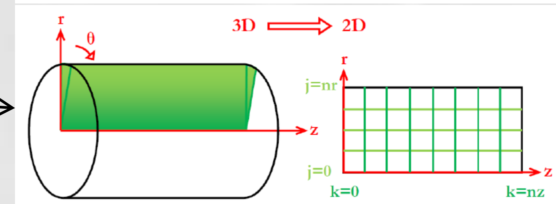
Plasma evolution

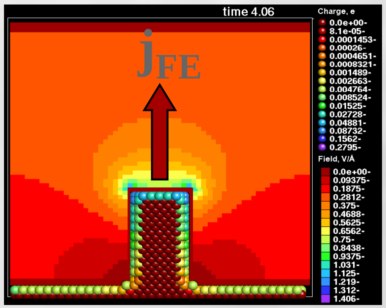
Corresponding to experiment...

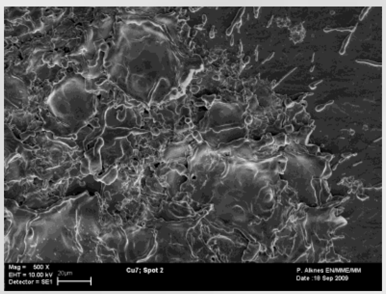
- Up to now we have electrostatic PIC-MCC codes:



- 1d3v
- 2D-model

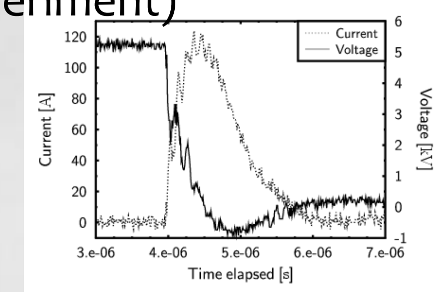


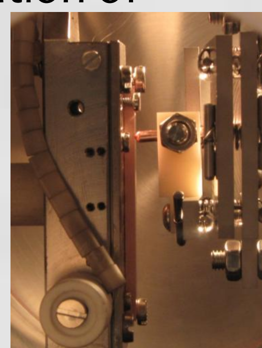




- Provide us with a link between

1. Micro- & macroscopic surface processes: Triggering (nano-scale) → plasma → crater formation (visible effect)
2. Theory & experiments: Using reasonable physical assumptions (theory), the aim is to predict the evolution of measurable quantities (experiment)

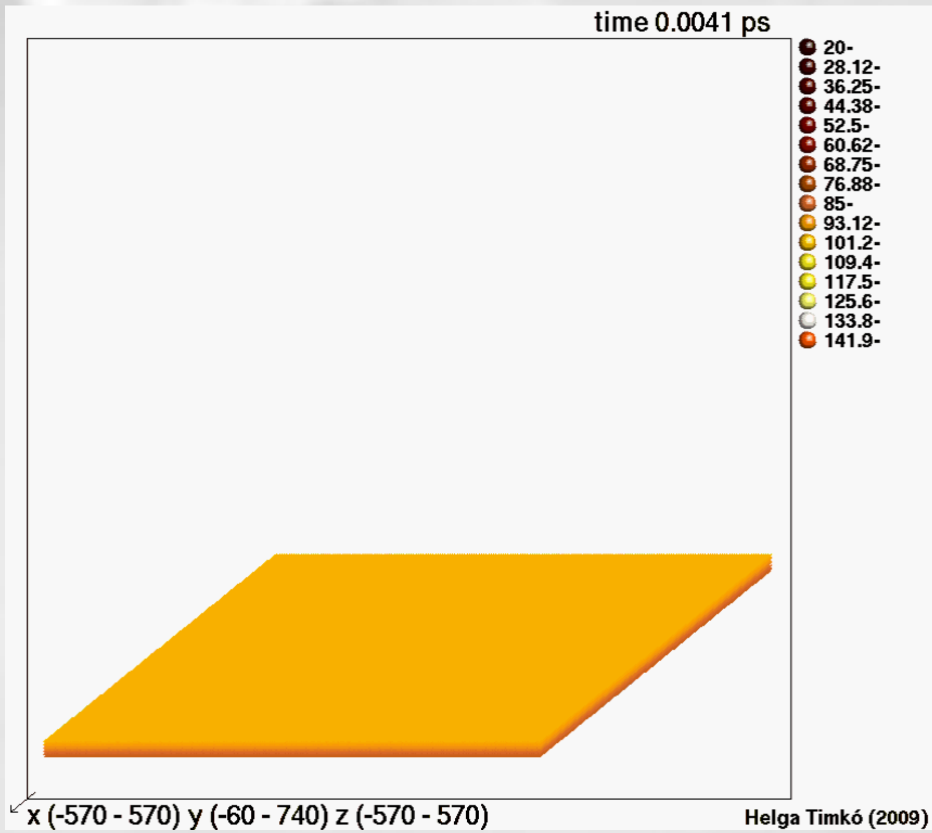




H. Timko, K. Matyash, R. Schneider, F. Djurabekova, K. Nordlund, A. Hansen, A. Descoeudres, J. Kovermann, A. Grudiev, W. Wuensch, S. Calatroni, and M. Taborelli , *Contrib. Plasma Phys.* 51, 5-21 (2011)

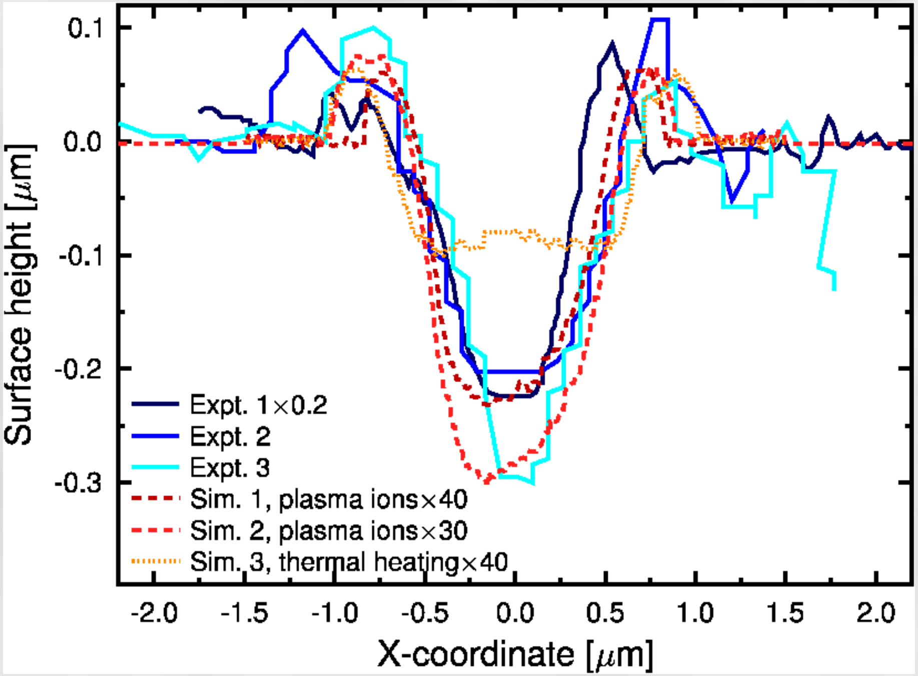
Classical MD simulations of sparks on Cu

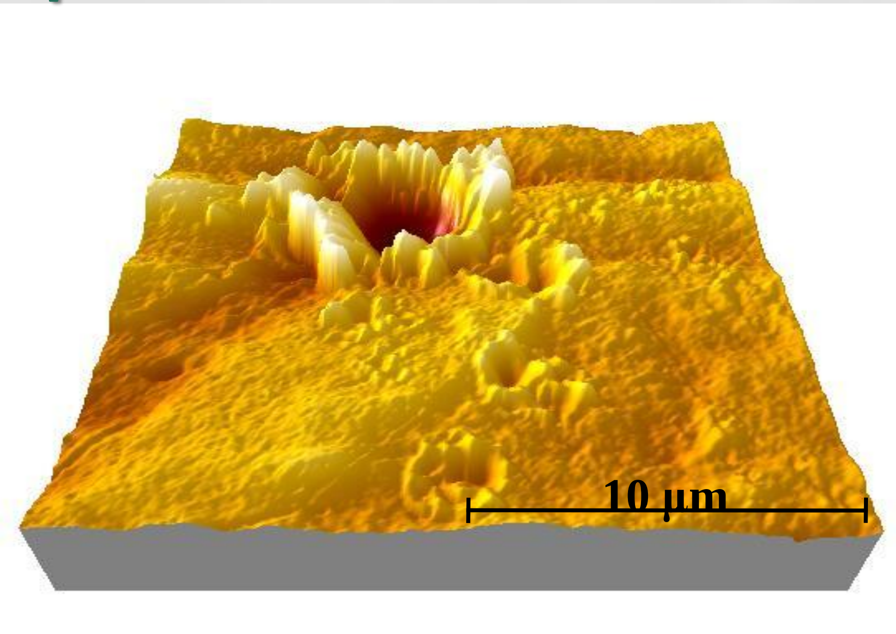
- MD simulations of surface bombardment on a given area *A*
  - Ion flux and energy distribution corresponded *exactly* to that from PIC simulations!

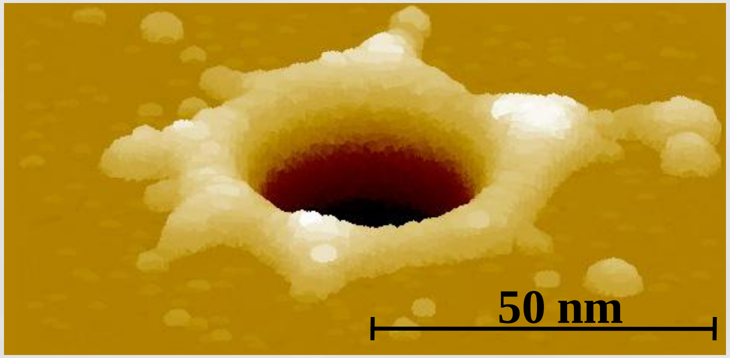


Comparison to experiment

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







H. Timko, F. Djurabekova et al., Mechanism of surface modification from the arc plasma-surface interaction in Cu, Phys. Rev. B 81, 184109 (2010).

Summary and perspectives

- Atomistic simulations have already helped to cast light on the mysterious behavior of metal surfaces in presence of high electric fields:
  - Charging of surface induces the tensile stress
  - The irregularities in the surface can concentrate the stress
  - The protrusions/intrusions can initiate the formation of field emitters -> plasma discharge -> surface damage!

- **In future**:
  - More mechanisms are to be discovered and stronger connections to the experiment to be established
    - Atomistic simulations <-> stochastic model <–> experimental data
    - This will help to design a metal alloy/composite/surface treatment to keep the breakdown rate within desirable limits

Thank you for your attention