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HIP

Multiphysics simulations of onset of vacuum electrical breakdowns

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University of Helsinki
Finland

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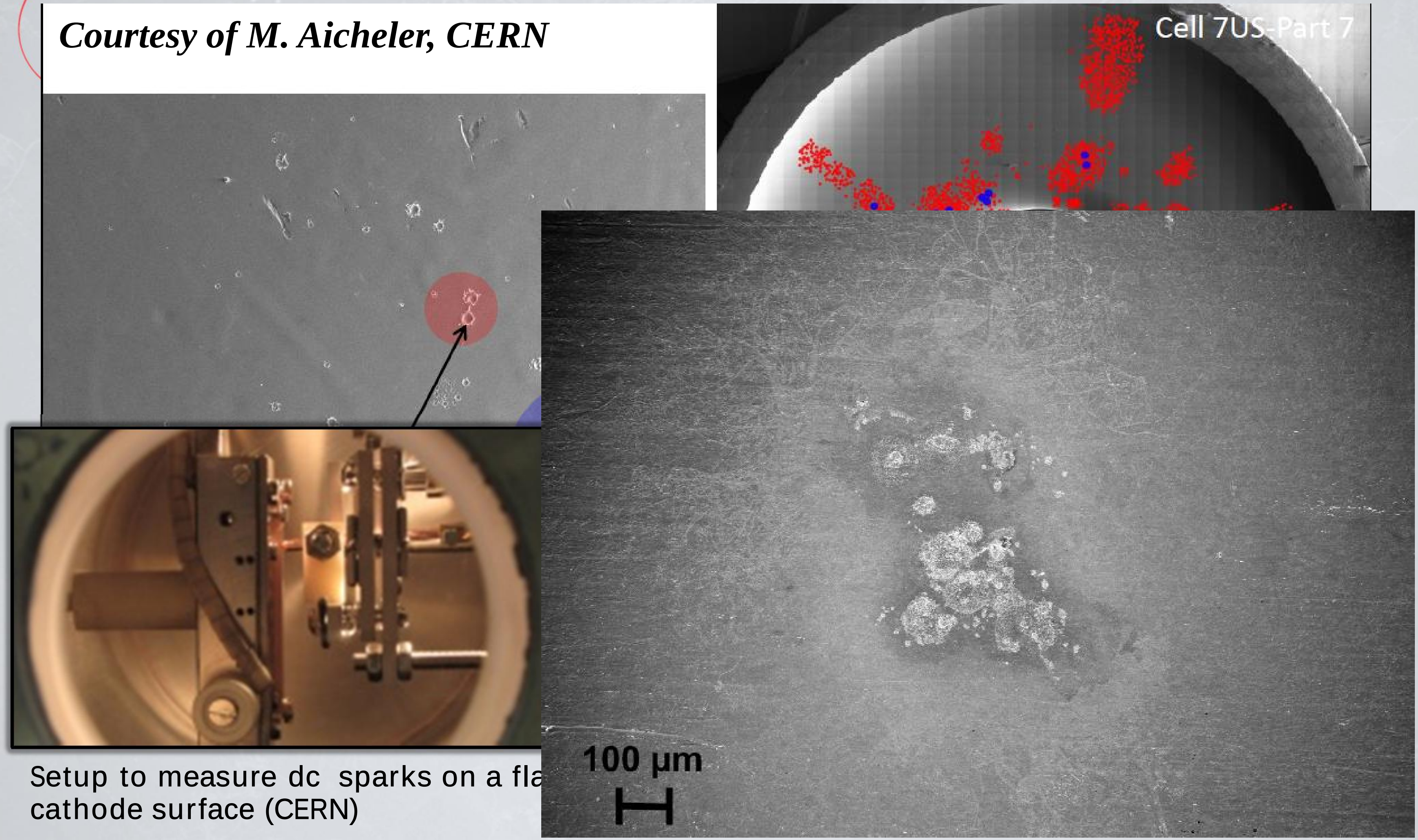
Motivation:

Electrical breakdowns in high gradient AS

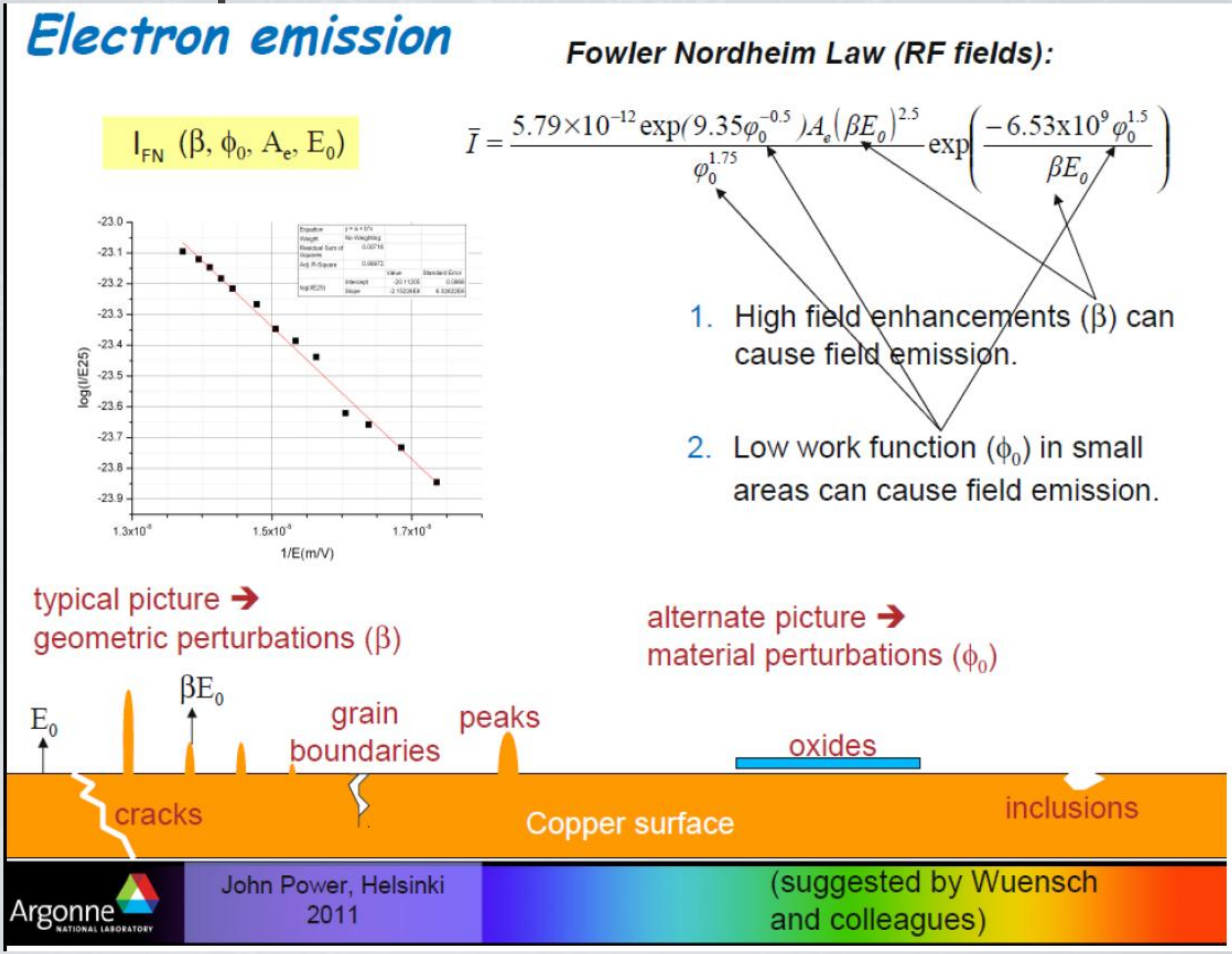


Courtesy of M. Aicheler, CERN

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

Important insight from experiments at CERN

- There is always field emission current before a breakdown event.
  - To understand the mechanism how localized field emitting spots form under the electric field might help to control the breakdown process.



Electron emission

Fowler Nordheim Law (RF fields):

$I_{FN}(\beta, \phi_0, A_e, E_0)$

$$\bar{I} = \frac{5.79\times10^{-12}\exp(9.35\varphi_0^{-0.5})A_e(\beta E_0)^{2.5}}{\varphi_0^{1.75}}\exp\left(\frac{-6.53\times10^{9}\varphi_0^{1.5}}{\beta E_0}\right)$$

1. High field enhancements (β) can cause field emission.
2. Low work function (ϕ_0) in small areas can cause field emission.

typical picture ➔
geometric perturbations (β)

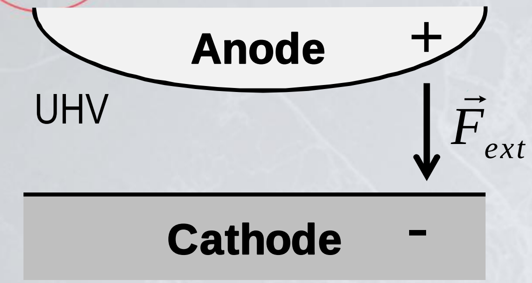
alternate picture ➔
material perturbations (ϕ_0)

John Power, Helsinki 2011

(suggested by Wuensch and colleagues)

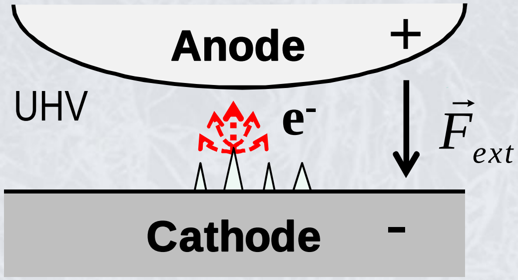
Vacuum arcing model

Stage 1



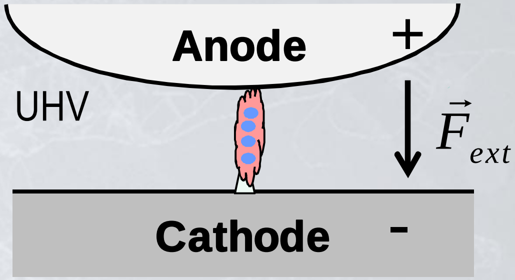
Test system e.g. at CERN; F_{ext} ramps up

Stage 2



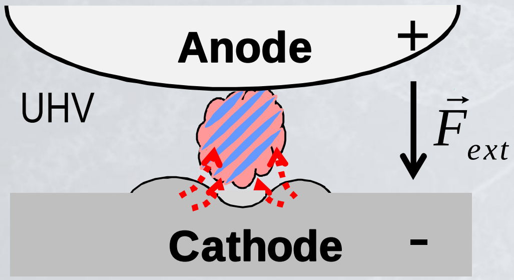
Tips grow on surface (seen as FE currents)

Stage 3



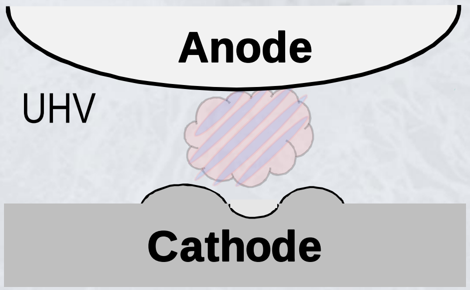
Plasma onset: FE currents, FAE of atoms, tips burn out

Stage 4

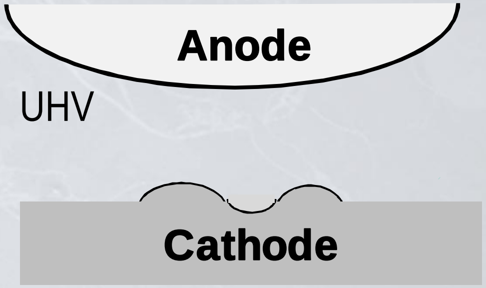


Plasma burning → cathode damage

Stage 5

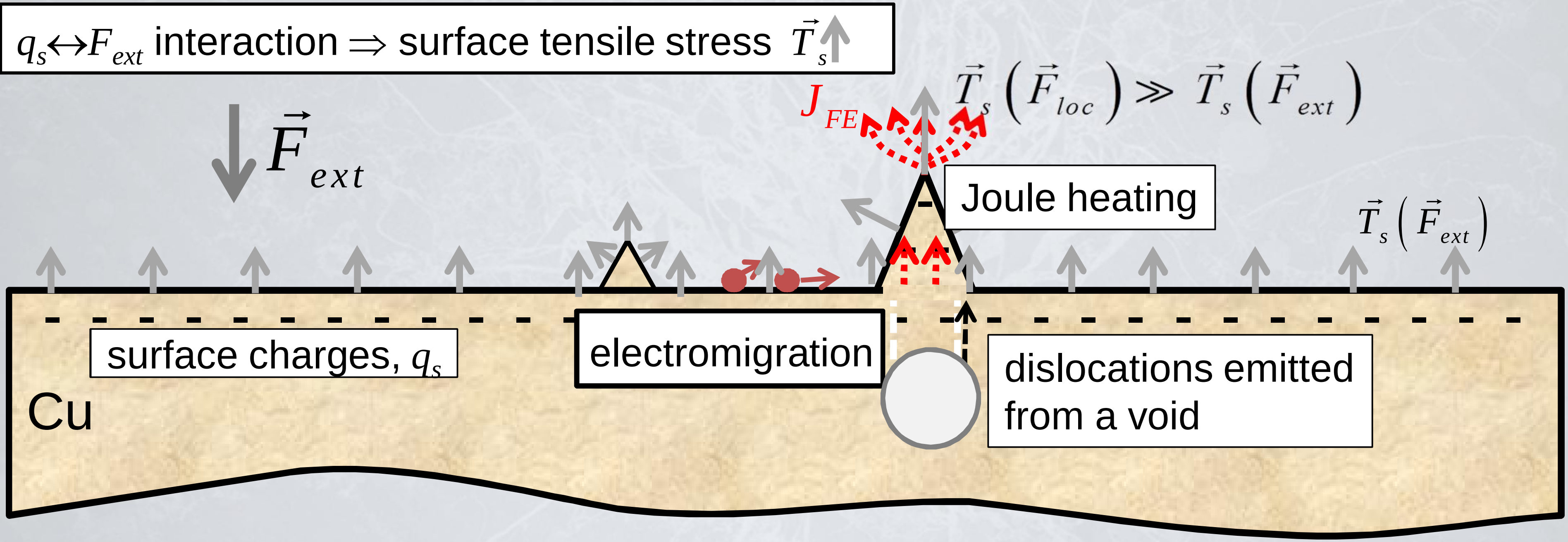


Extinction of energy, plasma burns out



Final damage remains, observed experimentally

Stage 1: onset of field emitters



$q_s \leftrightarrow F_{ext}$ interaction $\Rightarrow$ surface tensile stress $\vec{T}_s$

Joule heating

surface charges, q_s

electromigration

dislocations emitted from a void

Multiscale multiphysics model

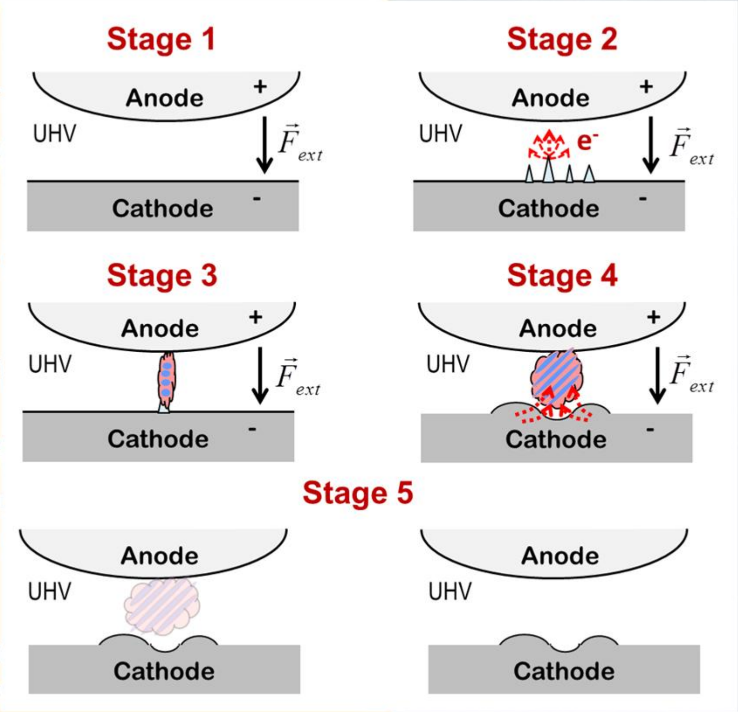
Stage 1 Charge on surface atoms **Method:** SIESTA (DFT), helmod (ED-MD)	~few fs
Stage 2a Onset of FE tip growth: Dislocation-mediated mechanism of surface protrusions **Method:** Comsol (FEM), parcas (MD), helmod	~few ns
Stage 2b Long time evolution of surface morphology affected by surface charge **Method:** kimocs (Kinetic Monte Carlo)	~10s ns
Stage 3 Field assisted evaporation of atoms & Joule heating, electromigration due to FE currents **Method:** helmod (ED-MD)	~ s/hs
Stage 4 Plasma evolution **Method:** Arc-pic (Particle-in-Cell)	~ s/min
Stage 5 Surface damage due to intense ion bombardment from plasma and heating by FE currents **Method:** Arc MD	~100s ns

ultiphysics model

Stage 1 Charge on
Method: SIESTA (DF

Stage 2a Onset of
Dislocation-mediate
surface protrusions
Method: Comsol (FEM
helmod

Stage 2b Long tim
surface morphology
surface charge
Method: kimocs (Kin



Stage 3 Field assisted evaporation of
ns & Jo ctromigr
to FE c

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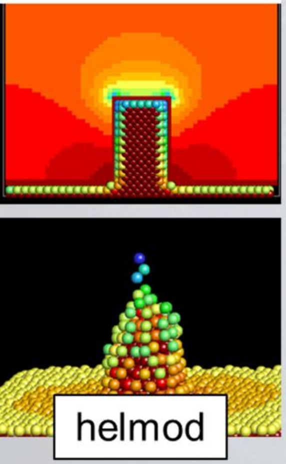
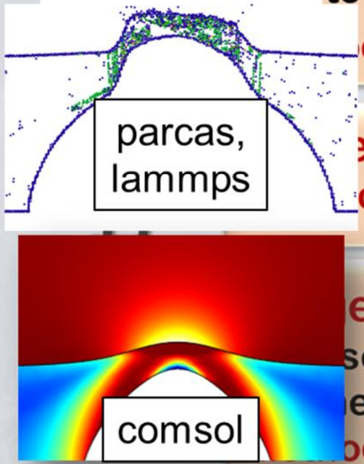
Stage 1



helmod

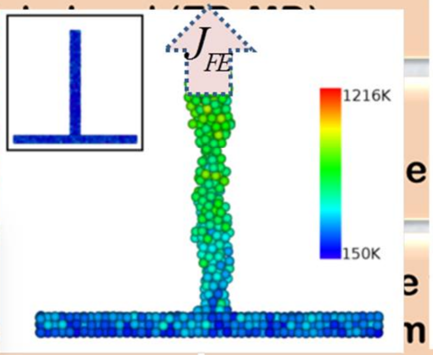
Stage 2



parcas, lammps

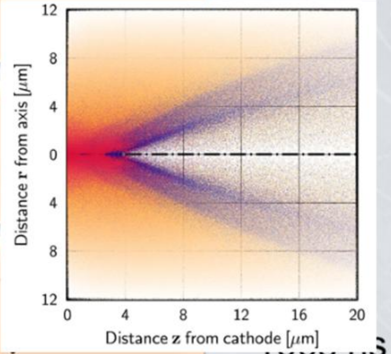
comsol

Stage 3



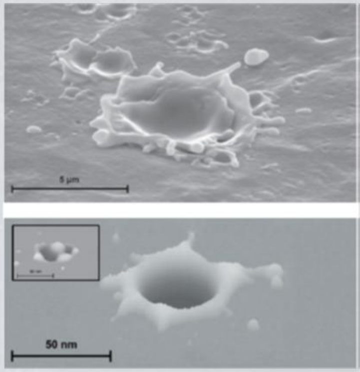
helmod

Stage 4



Arc-PIC

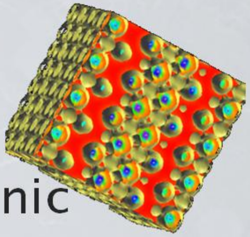
Stage 5



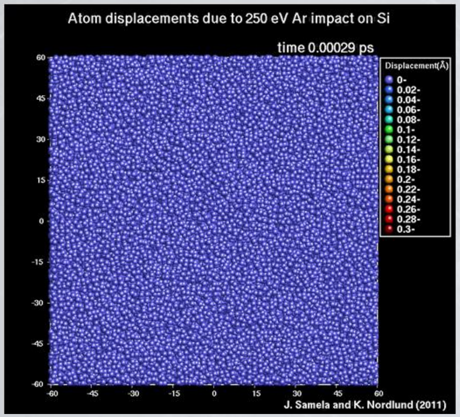
Arc-MD

Tools in use:

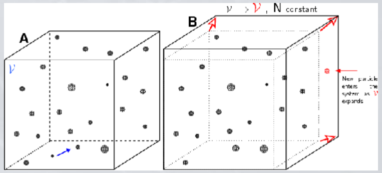
- In our group we use all main atomic-level simulation methods:
  - Density functional theory (DFT)
    - Solving Schrödinger equation to get electronic structure of atomic system



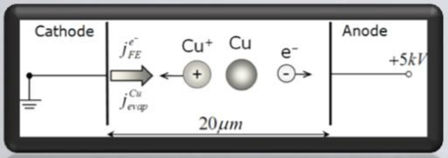
  - Molecular dynamics (MD)
    - Simulation of atom motion, classically and by DFT
    - Hybrid ED-MD (*helmod*) approach



  - Kinetic Monte Carlo (KMC)
    - Simulation of atom or defect migration in time

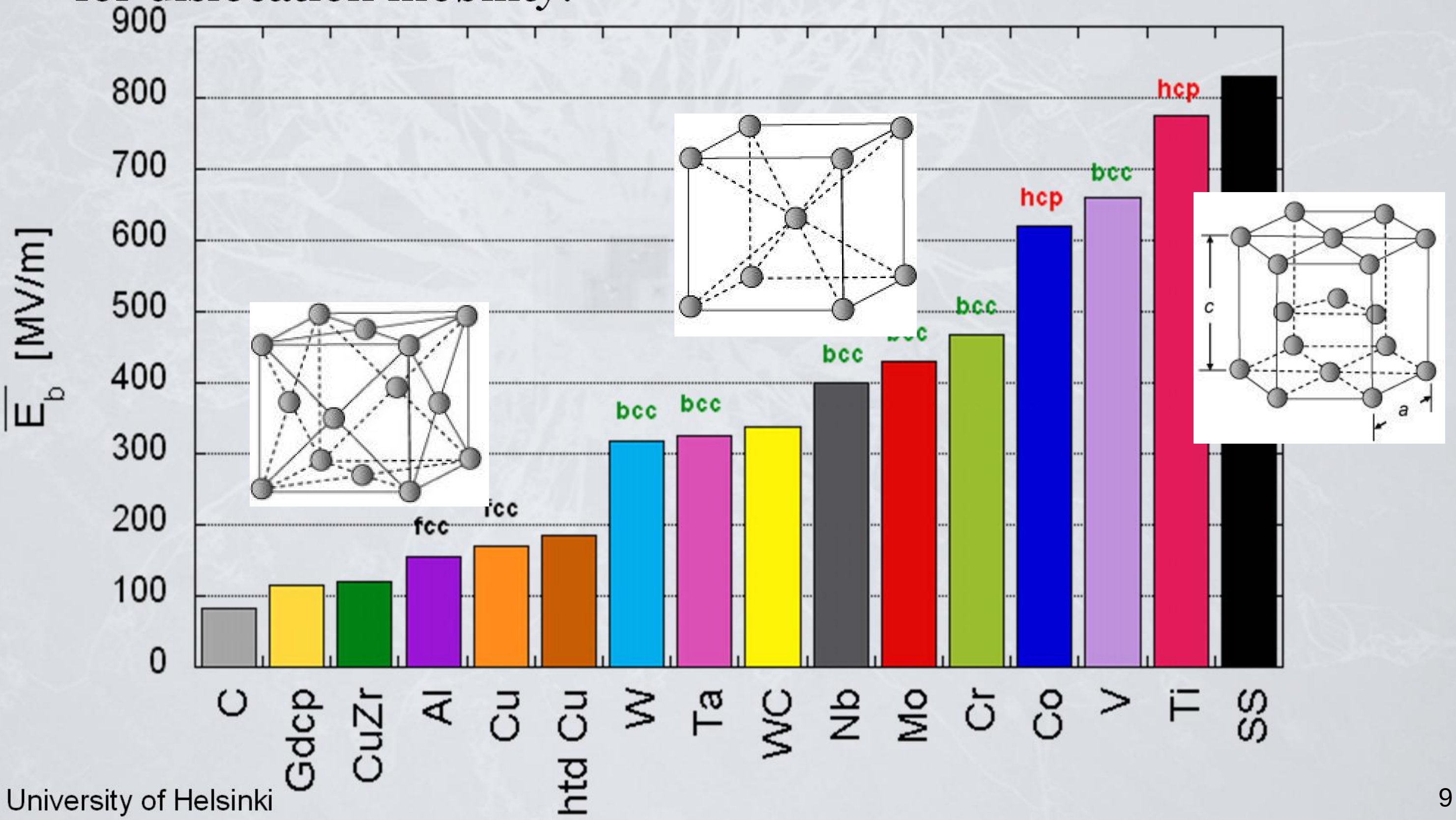


  - Simulations of plasma-wall interactions
    - Simulation of plasma particle interactions with surfaces



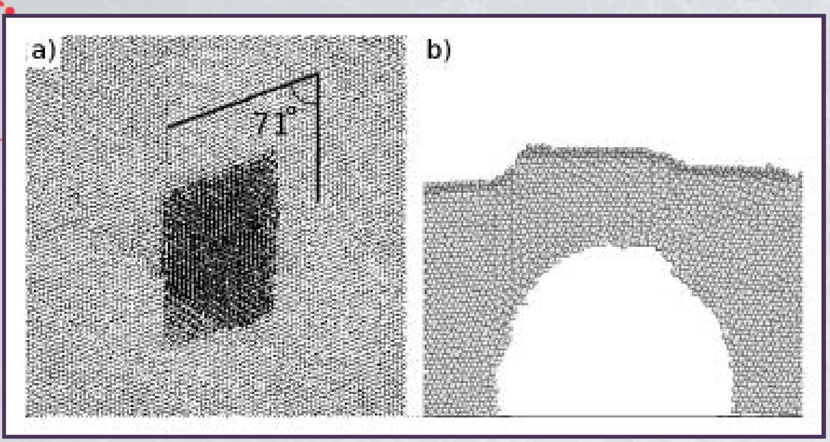
What are the field emitters?
Why do we look for dislocations?

- The dislocation motion is strongly bound to the atomic structure of metals. In FCC (face-centered cubic) the dislocation are the most mobile and HCP (hexagonal close-packed) are the hardest for dislocation mobility.

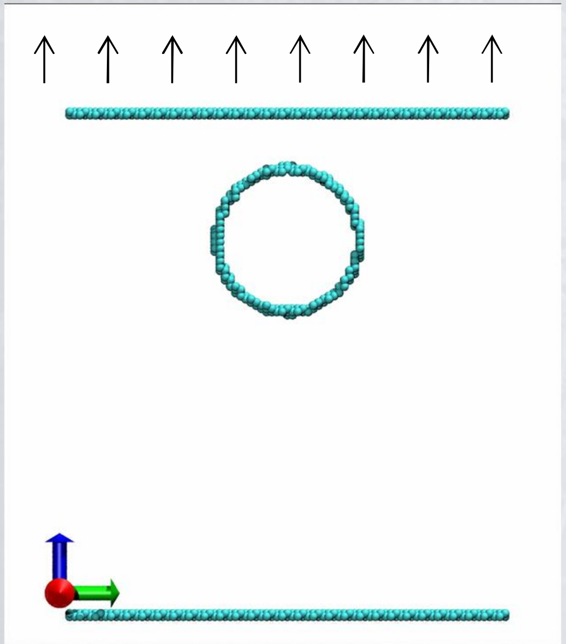


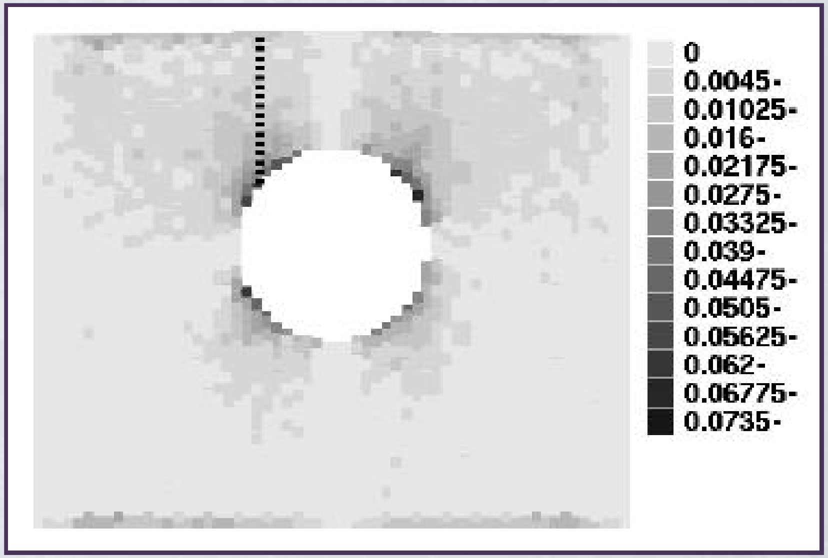
A. Descoeudres, F. Djurabekova, and K. Nordlund, DC Breakdown experiments with cobalt electrodes, CLIC-Note XXX, 1 (2010).

A void hypothesis as a lattice irregularity



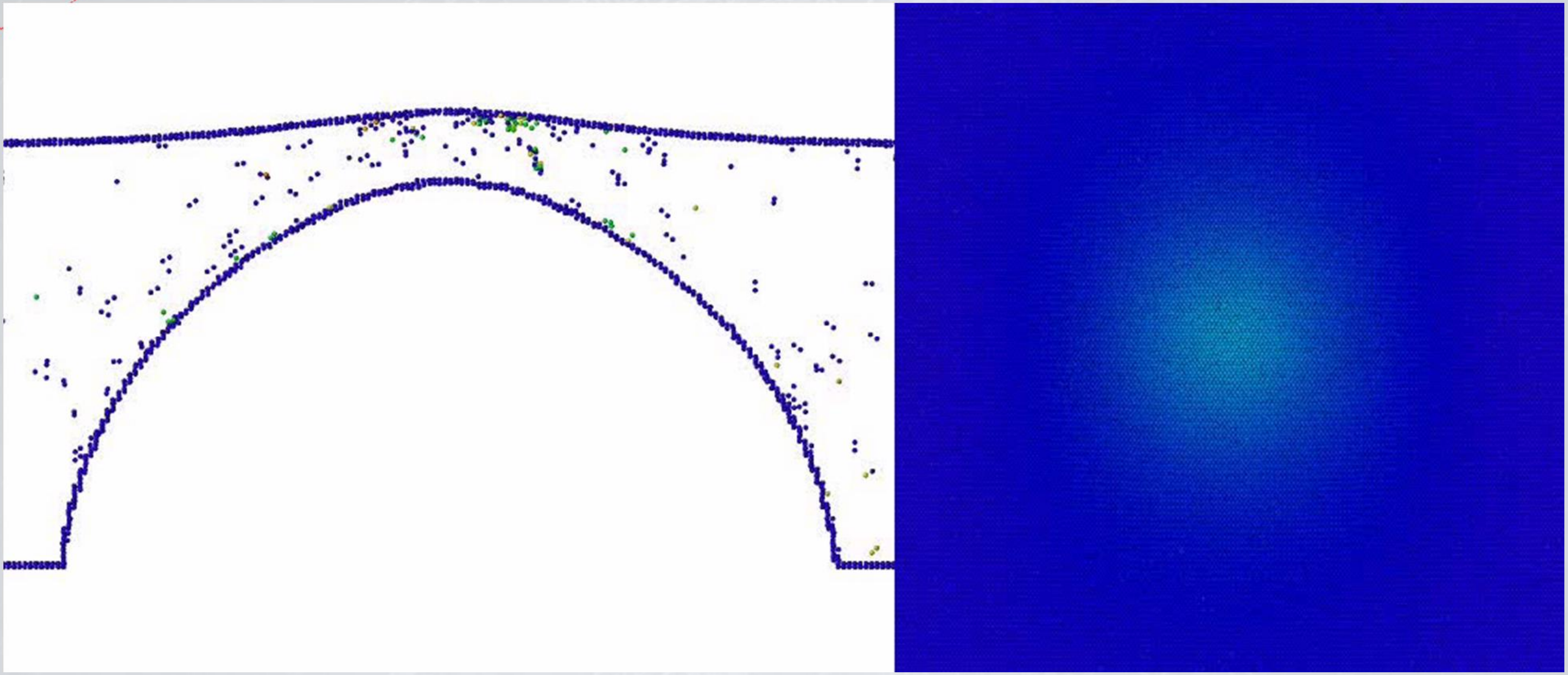
- We simulated a void near {110} Cu surface , when the high tensile stress is applied on the surface. Bottom is fixed, lateral boundary allowed to move in z direction.





A. Pohjonen, F. Djurabekova, et al, JAP. 110, 023509 (2011).

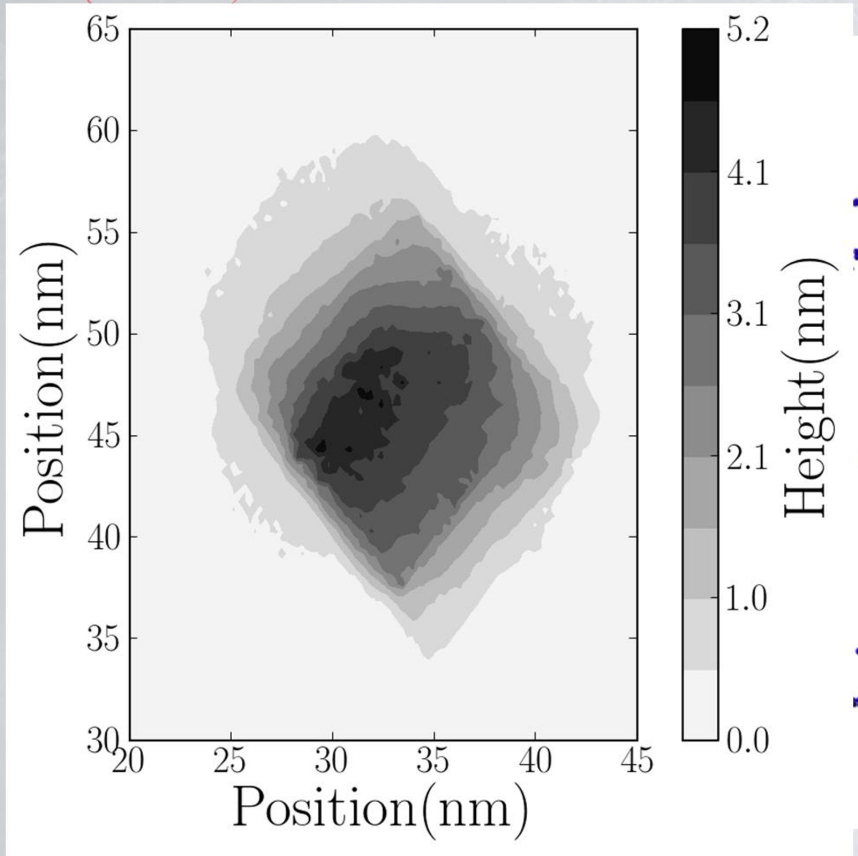
Switching on the electric field above the surface

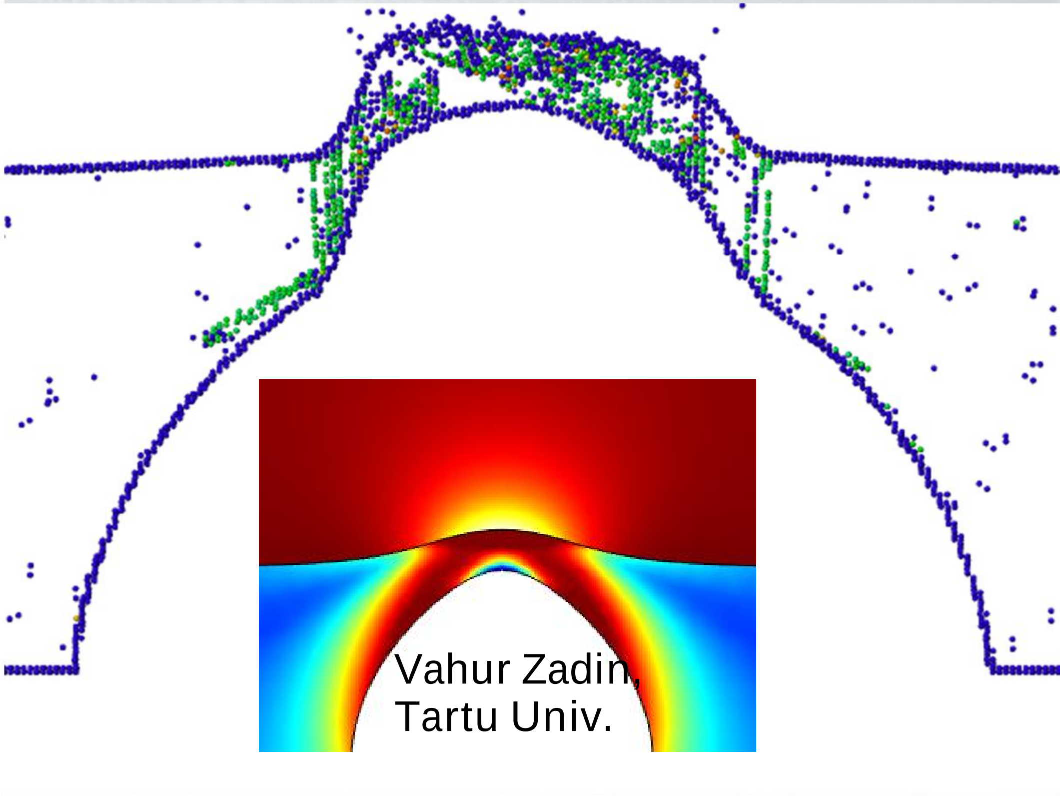


- We also analyzed the behavior of a void under tensile stress due to the electric field (Simulations now done with the *helmod* code, where the electric field effect is accounted explicitly)

[A. S. Pohjonen, S. Parviainen, T. Muranaka, and F. Djurabekova, JAP 114, 033519 (2013)]

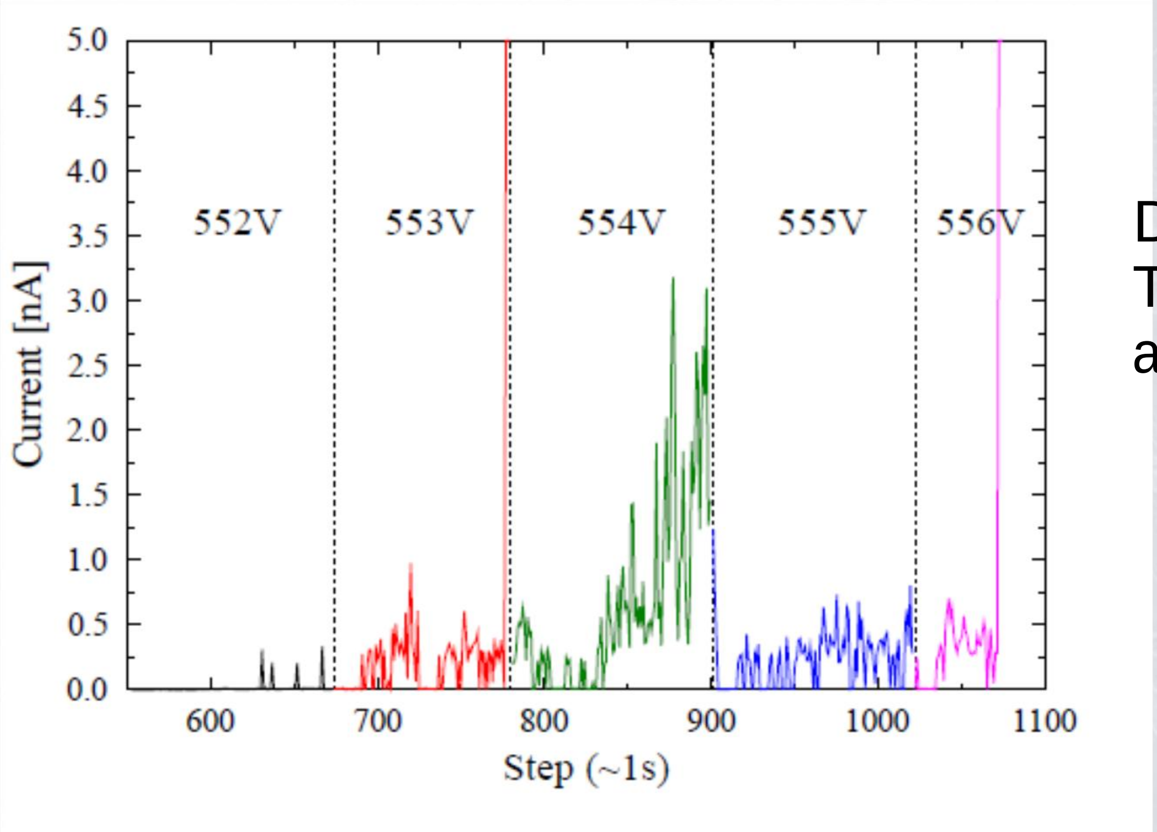
“Catastrophic” growth of a protrusion at the void



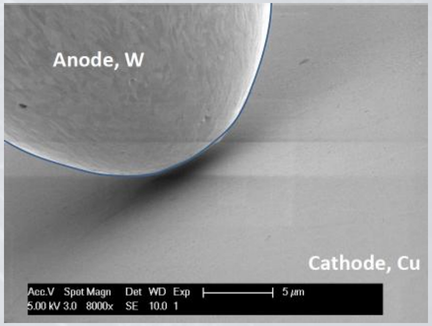

Vahur Zadin, Tartu Univ.

- . the top view and a slice of the system at time t = 130 ps when the fully developed protrusion is clearly visible.

Field emission current



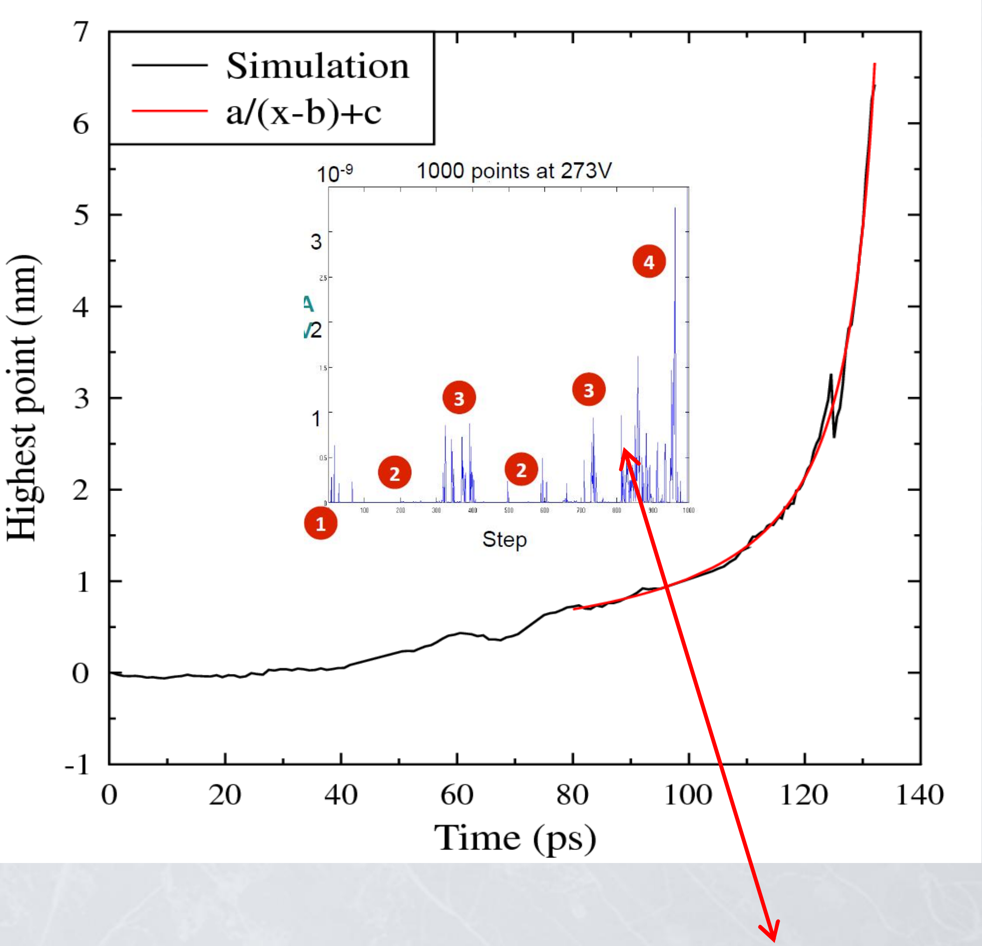
Data courtesy of Tomoko Muranaka at Uppsala Univ.



- Field emission current from a Cu sample at different applied voltages. The current increases even though the voltage remains unchanged. This indicates that surface modification occurs, which increases the field enhancement/the emission current.

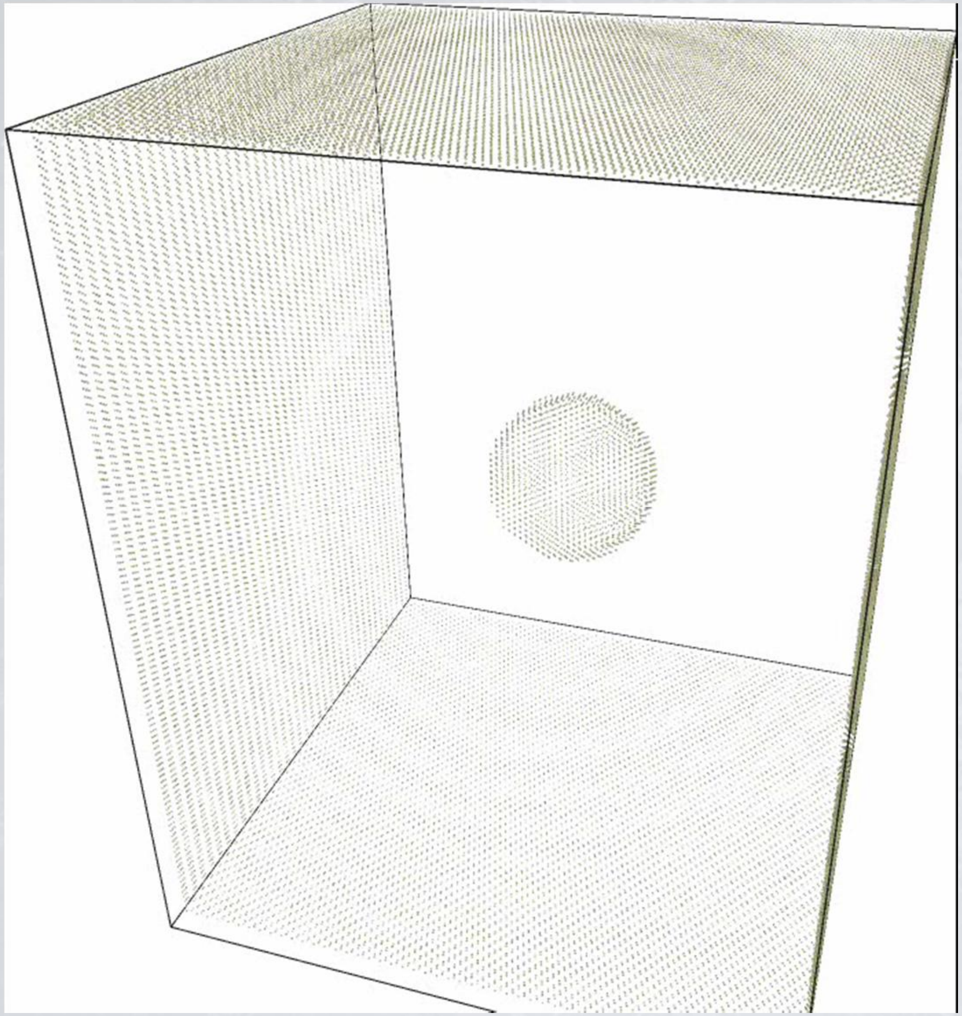
The “catastrophic” growth of a protrusion in the presence of the field

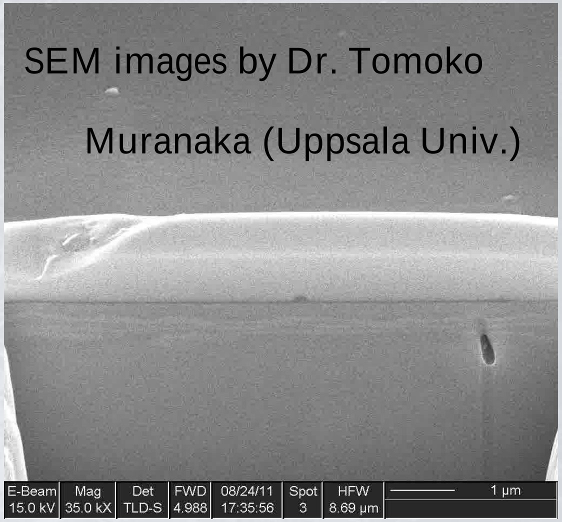
- The analysis of the protrusion height increase shows an asymptotic character. Once it starts growing, the self-reinforcing effect of the field enhancement around the tip of the protrusion causes the increase of its height in the ”catastrophic” manner



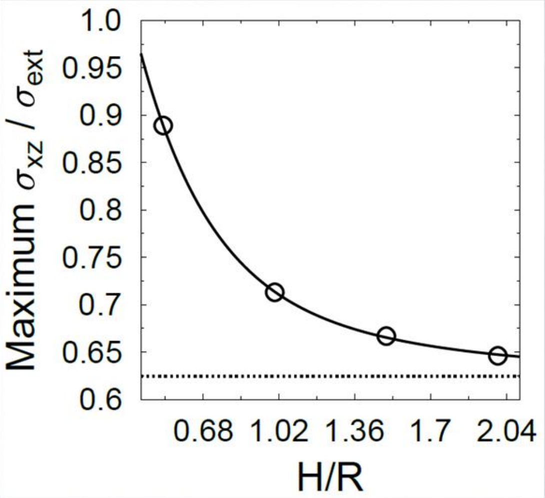
Experiment by Tomoko Muranaka, CERN

Deeper under the surface





SEM images by Dr. Tomoko Muranaka (Uppsala Univ.)



- Now we placed the void 4 void radii below the surface. A simulation was performed without actual electric field calculations

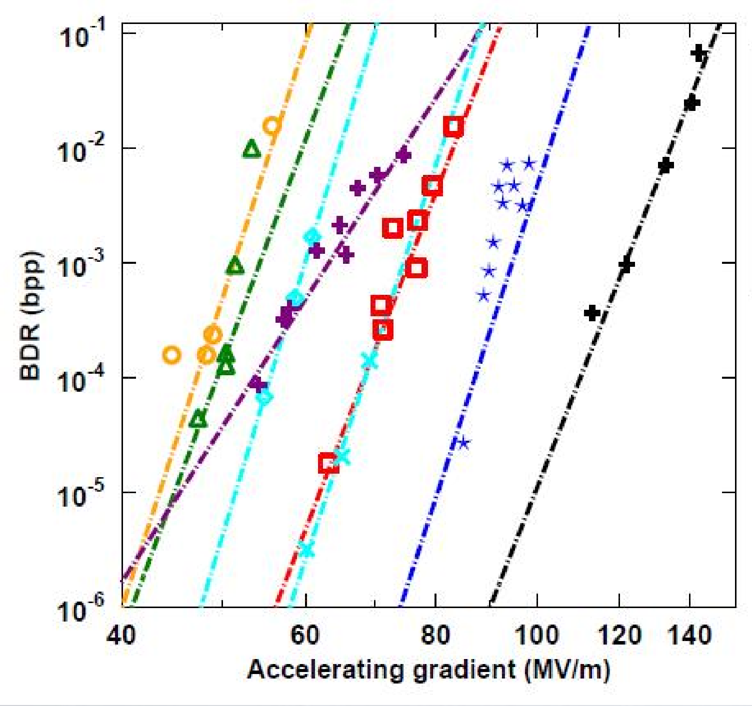
Dislocation-based model for electric field dependence

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

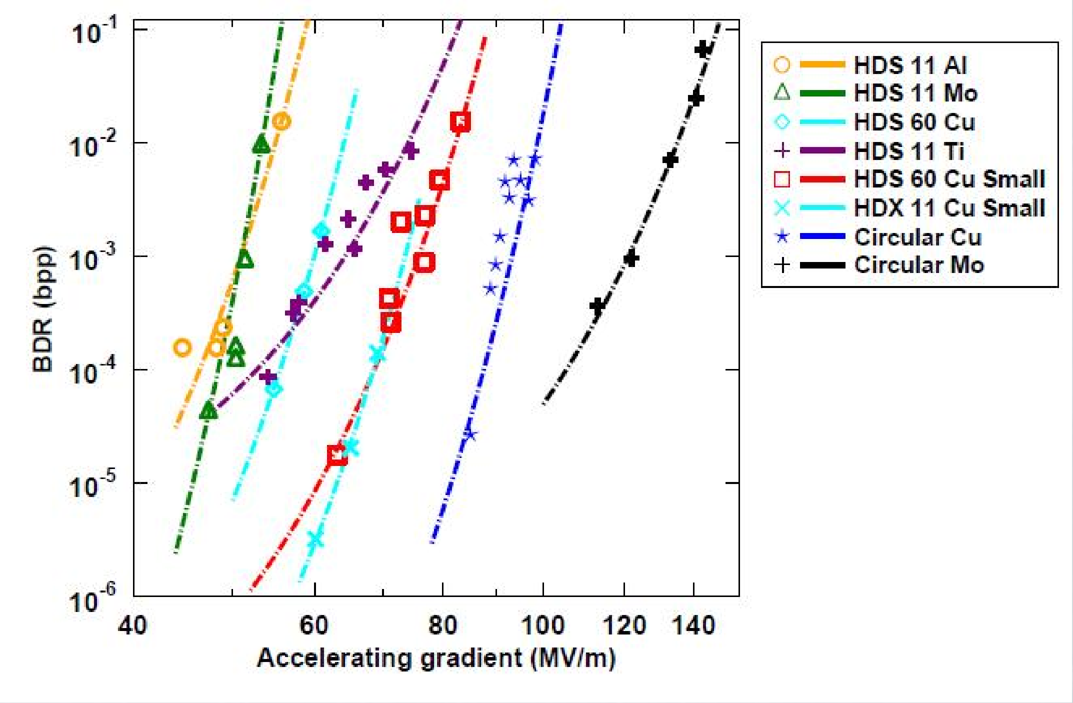
$$BDR = AE^{29}$$

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

Power law fit



Stress model fit



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

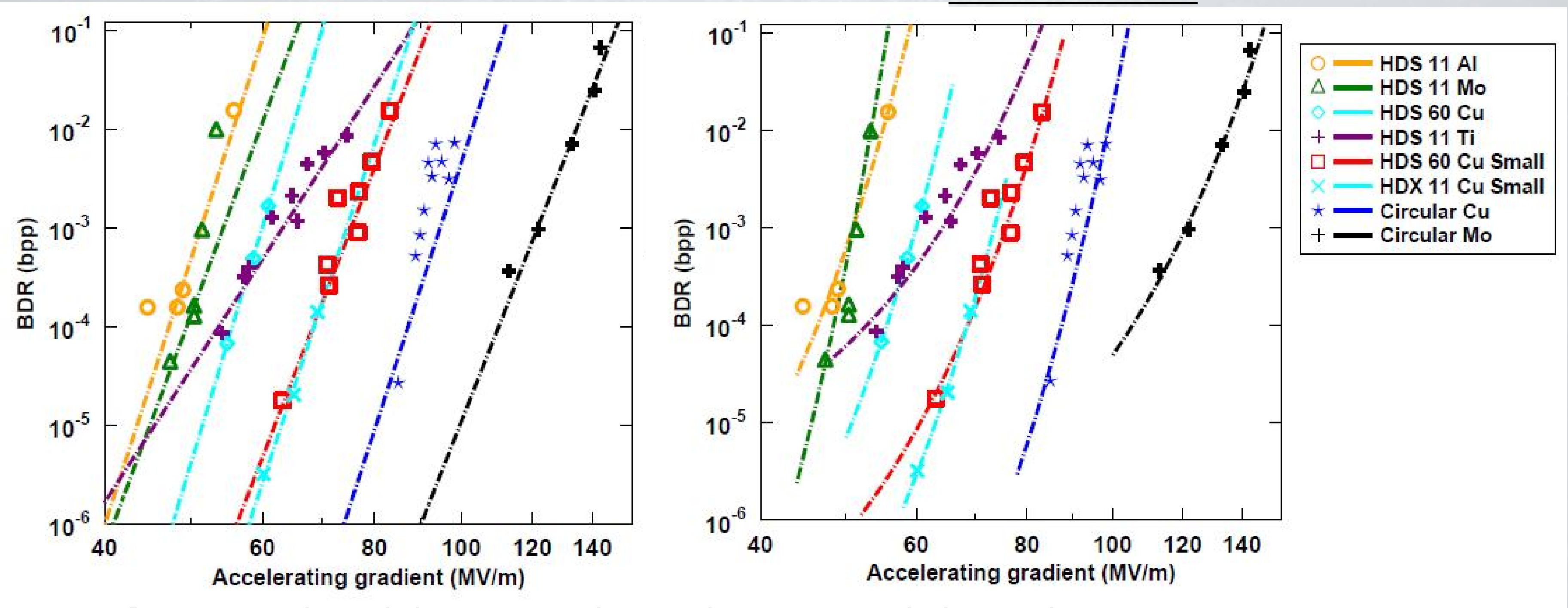
K. Nordlund and F. Djurabekova, Phys. Rev. ST-AB 15, 071002 (2012).

Dislocation-based model for electric field dependence

$$BDR \propto c_0 e^{-(E^f - \varepsilon_0 E^2 \Delta V)/kT}$$

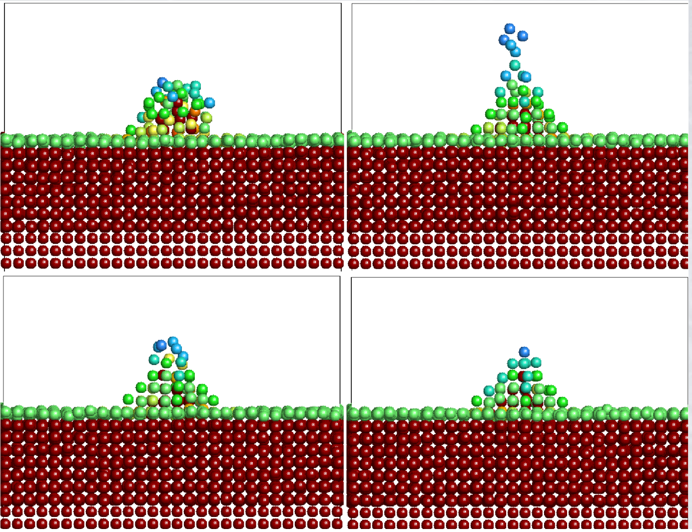
$$BDR = A e^{\varepsilon_0 E^2 \Delta V / kT} = c_0 e^{-E^f / kT} e^{\varepsilon_0 E^2 \Delta V / kT}$$

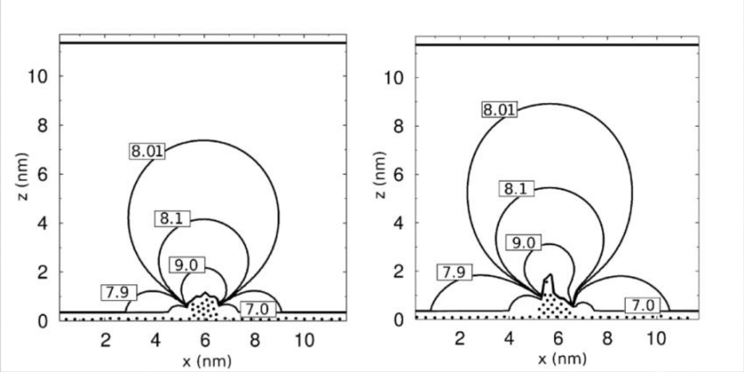
- Now to test the relevance of this, we fit the experimental data
- The result is:


Power law fit **Stress model fit**

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

Evolution of a tip placed on Cu surface



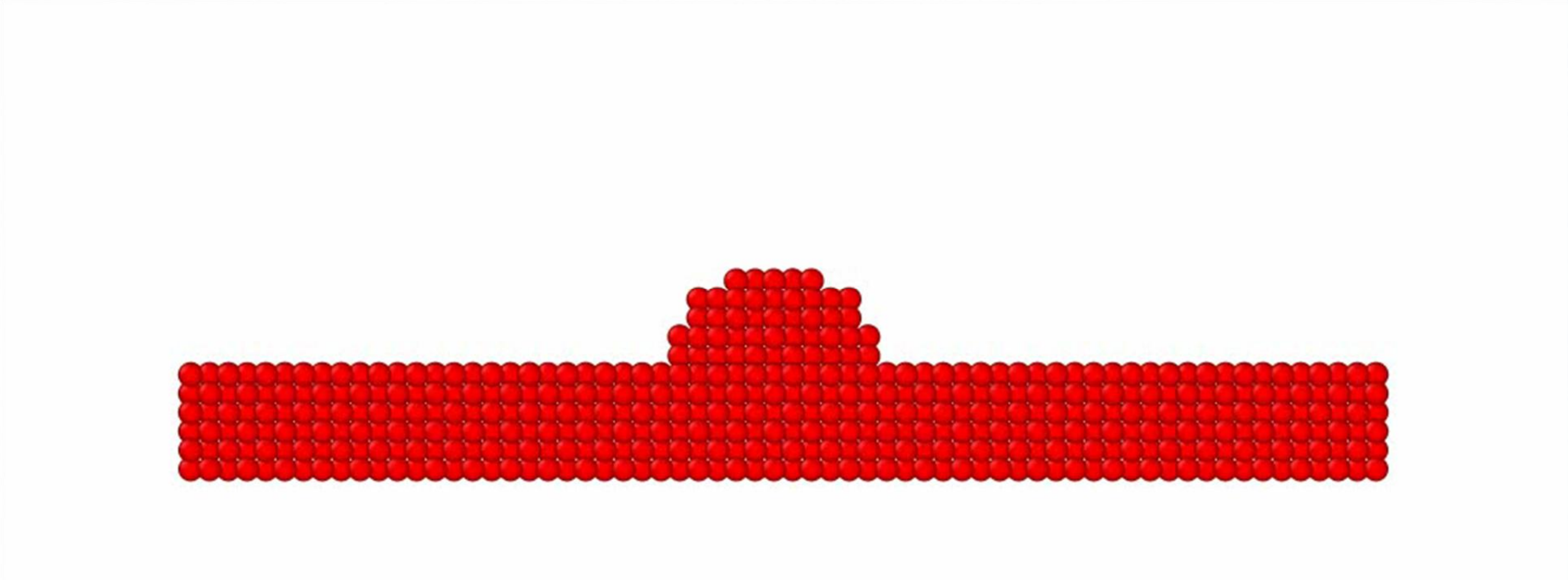


- We developed a novel approach *helmod* code (hybrid ED-MD code, based on classical MD code)to follow the dynamic evolution of partial charge on surface atoms by combining the MD and classical ED (solving Laplace equation)
- The dynamics of atom charges follows the shape of electric field distortion on tips on the surface
- Temperature on the surface tips is sufficient => atom evaporation enhanced by the field can supply neutrals to build up the plasma densities above surface.

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

Evolution of a surface tip

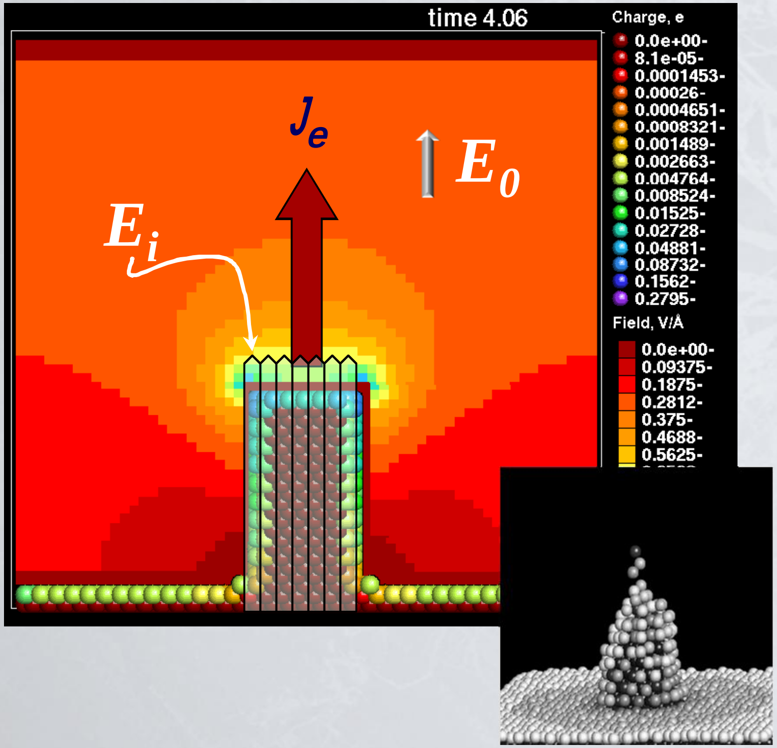
- Applied field F_{ext}=10 GV/m, the ambient temperature T=500 K
- Ramping rate $\Delta F/\Delta t=0.05\ V/Å^{-1}fs^{-1/2}$



Fowler-Nordheim approximation for field emission

- Every atomic column produces the current dependent on the field above the column. The current from the tip is an average over all the columns.

$$J(E,T,\phi) = \lambda_T(E,T,\phi)J_0(E,\phi)$$



$$\begin{cases} J_0(E,\phi) = \dfrac{aE^2}{\phi}\exp\left(-\dfrac{b\phi^{3/2}}{E}\right) \\ \lambda_T(E,T,\phi) = \dfrac{\pi k_B T / d_T(E,\phi)}{\sin\left(\pi k_B T\right) / d_T(E,\phi)} \end{cases}$$

Fowler-Nordheim constants:

$$a = \frac{e^2}{8\pi h_P} = 1.541\frac{\mathrm{A}\cdot\mathrm{V}}{\mathrm{eV}^2}$$

$$b = \frac{8\pi\sqrt{2m}}{3eh_P} = 6.831\frac{\mathrm{V}}{\mathrm{eV}^{3/2}\ \mathrm{nm}}$$

The heat conduction from the tip has been implemented into MD

- The heat conduction from the tip has been implemented into *helmod* by solving the heat conduction equation

$$\frac{\partial T(x,t)}{\partial t} = \frac{1}{C_V}\left(\rho\big(T(x,t)\big)\,J(x)^2 + K_e(T)\frac{\partial^2 T(x,t)}{\partial x^2}\right)$$

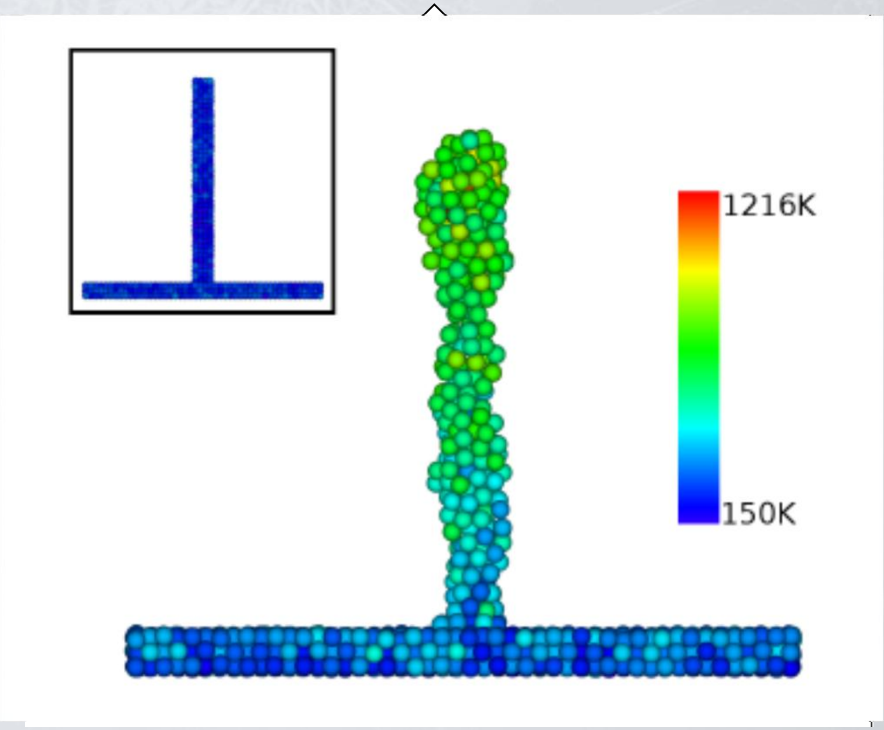
Here C_V volumetric heat capacity. *Phonons are implicitly present in classical MD*. Electron thermal conductivity is given by the Wiedemann-Franz law

$$K_e(T) = \frac{LT}{\rho(T)}$$

Where Lorenz number is found as

$$L = (\pi^2/3)(k_B^2) = 2.443\times10^{-8}\ \mathrm{W\Omega K^{-2}}$$

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



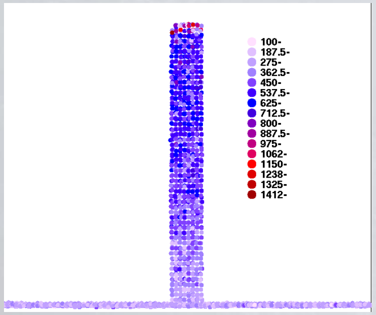
From tips to plasma:

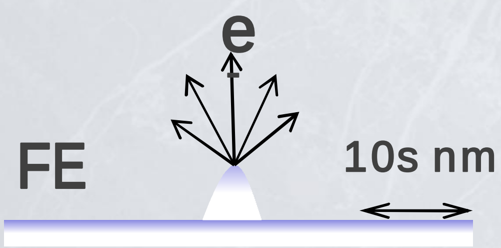
From FE to discharge currents

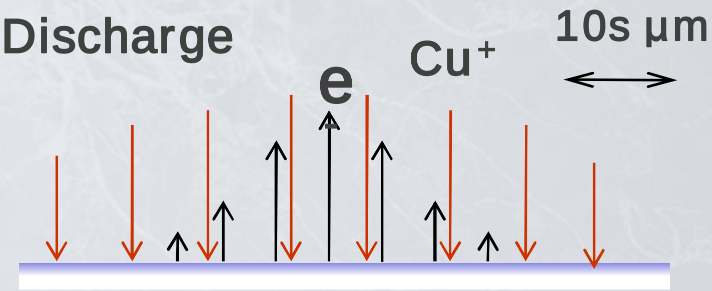
- In real life we can observe the full dynamic range of a vacuum discharge:
  - > 10s pA in ‘weak’ FE phase
  - Space charge limited ‘strong’ FE phase, typically ~ nA – μA
  - Discharge current, up to 10 – 100 A
- At the same time, the involved area changes:
  - Typically $10^{-20} – 10^{-14}$ m^2 for weak FE ⇒ R_{em} ~ 0.1 – 100 nm
  - During the discharge, the bombarded area has R ~ 10 – 100 μm

Up to 12 orders of magnitude difference

Up to 12 orders of magnitude difference

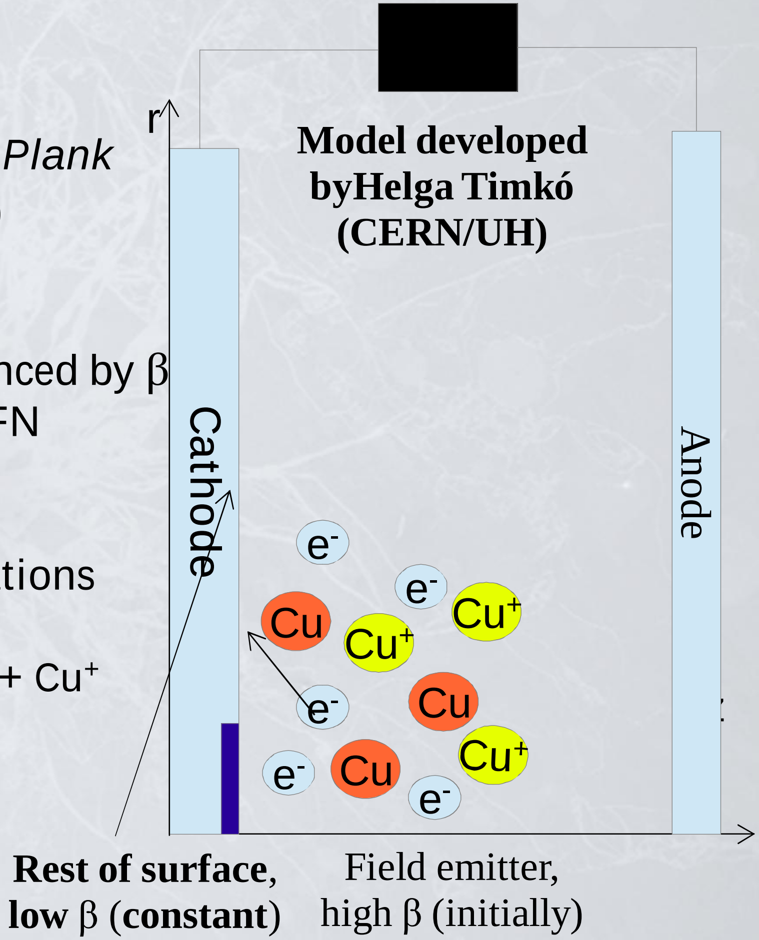






2D Arc-PIC in a nutshell

- 2d3v electrostatic PIC code with cylindrical symmetry
  - Particles: e^-, Cu, and Cu^+
  - Monte Carlo collision routines (*Max Plank Institute of Plasma Physics, K.Matyash*)
- Emission processes
  - Fowler-Nordheim field emission – enhanced by β
  - Simplified Cu evaporation – fraction of FN emission
  - Sputtering (*Yamamura & Tawara*)
  - Heat spike sputtering – from MD simulations
  - Secondary electron yield - constant
  - Ions only through impact: $e^- + Cu \rightarrow 2e^- + Cu^+$
- External RC circuit
  - Potential stored in capacitor
    - Drained by arc current



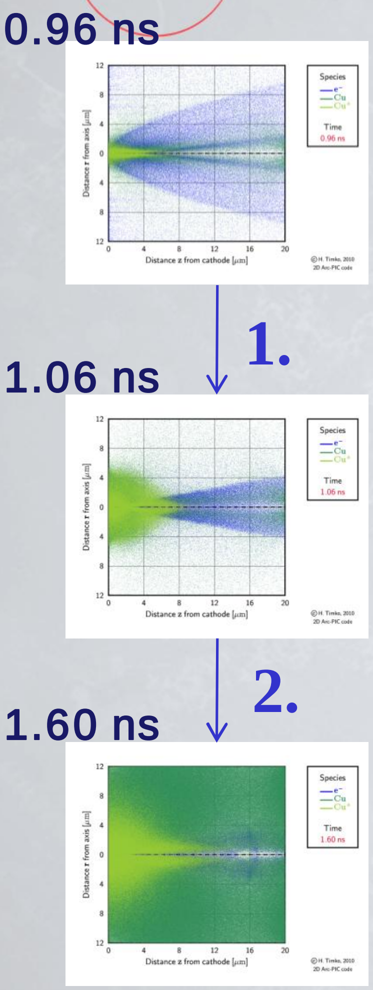
Model developed byHelga Timkó (CERN/UH)

Rest of surface, low β (constant)

Field emitter, high β (initially)

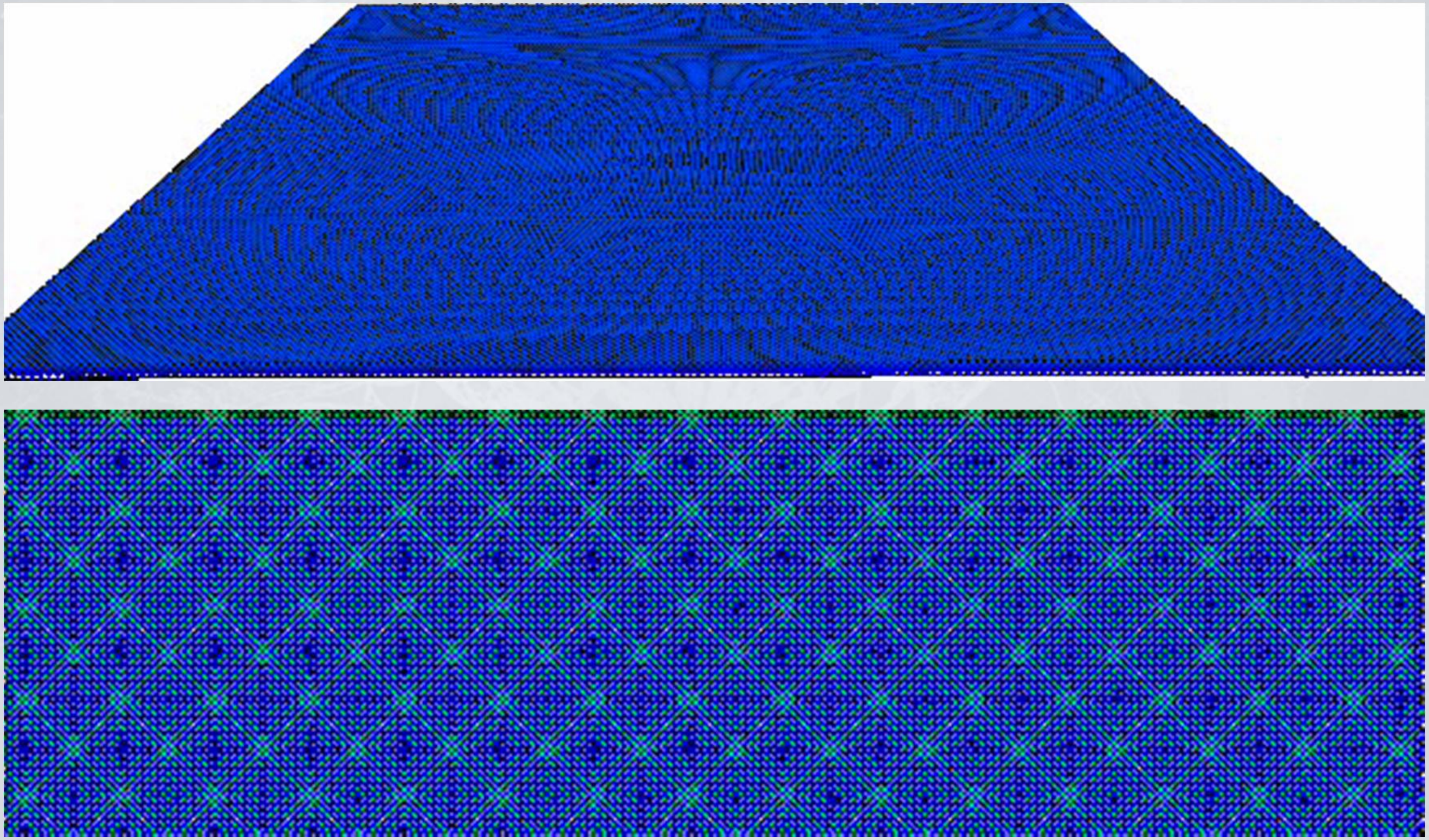
H. Timko et al. *Contrib. Plasma Phys. 5*1, 5-21 (2011)

Observations



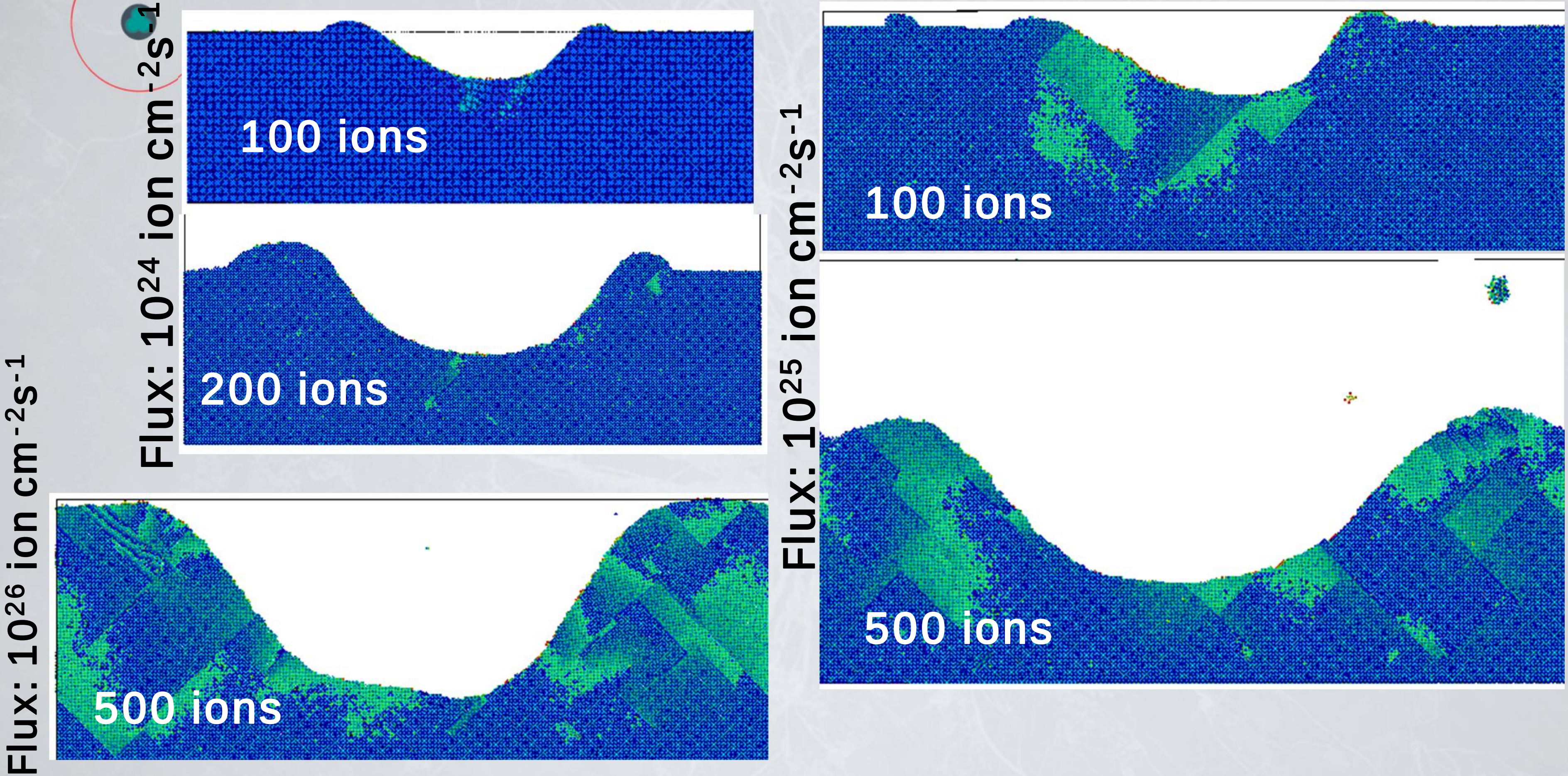
- Mostly cathode dominated phenomenon
- Although FE starts from a small area, the discharge plasma can involve a macroscopic area on the cathode
- Transitions seen:
  1. Transition from strong FE to a small discharge plasma
     - Sudden ionisation avalanche
     - A plasma sheath forms, the plasma becomes quasi-neutral
     - Focusing effect
  2. Transition from a surface-defined phase to a volume-defined phase
     - When neutrals fill the whole system
     - Self-maintaining
     - Macroscopic damage

Plasma impacts: Arc-MD simulations



- The impact of 200 ions with the flux of 10^{24} ions cm^{-2}s^{-1}
- Energy of ions 6 keV at RT

Changing fluxes

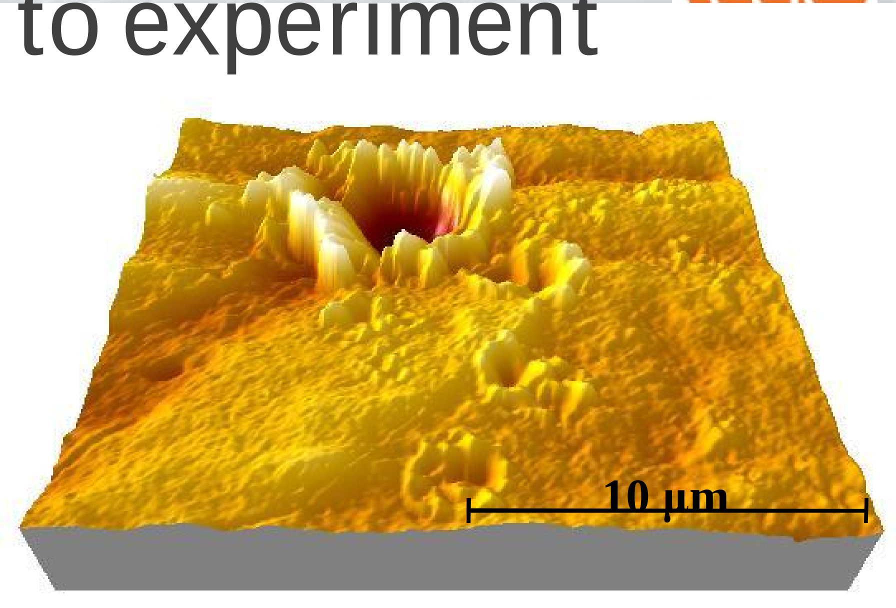


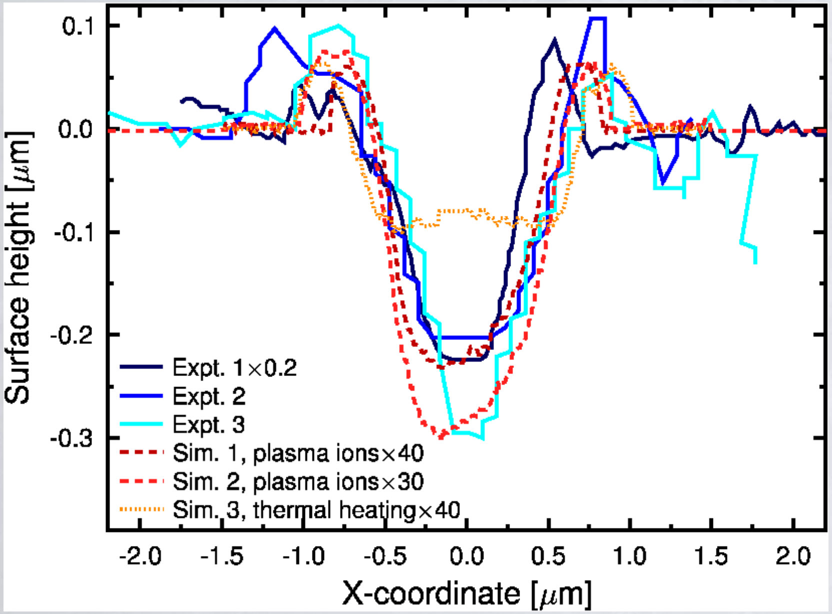
- Plastic deformations under the craters formed by plasma ions with different fluxes

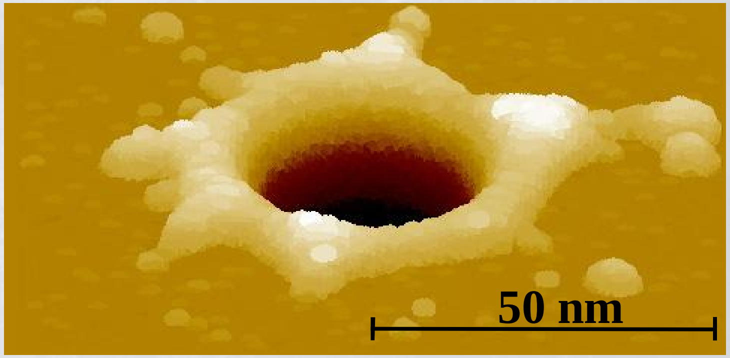
Comparison to experiment

- 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

- The model has been actively developed and gave many new insights in the physics of the plasma onset and surface damage
- The model underlines the importance of mechanical properties of metal surfaces
- The coupling of dislocation model and electric field effect resulted in “catastrophic” protrusion growth, which was not observed previously, but intuitively in line with field emission measurements from flat copper surfaces.
- Analysis of the surface damage after craters cooled down reveals the presence of significant structural defects, which can be analyzed for prediction of positioning of future breakdown spots.

Thanks to:

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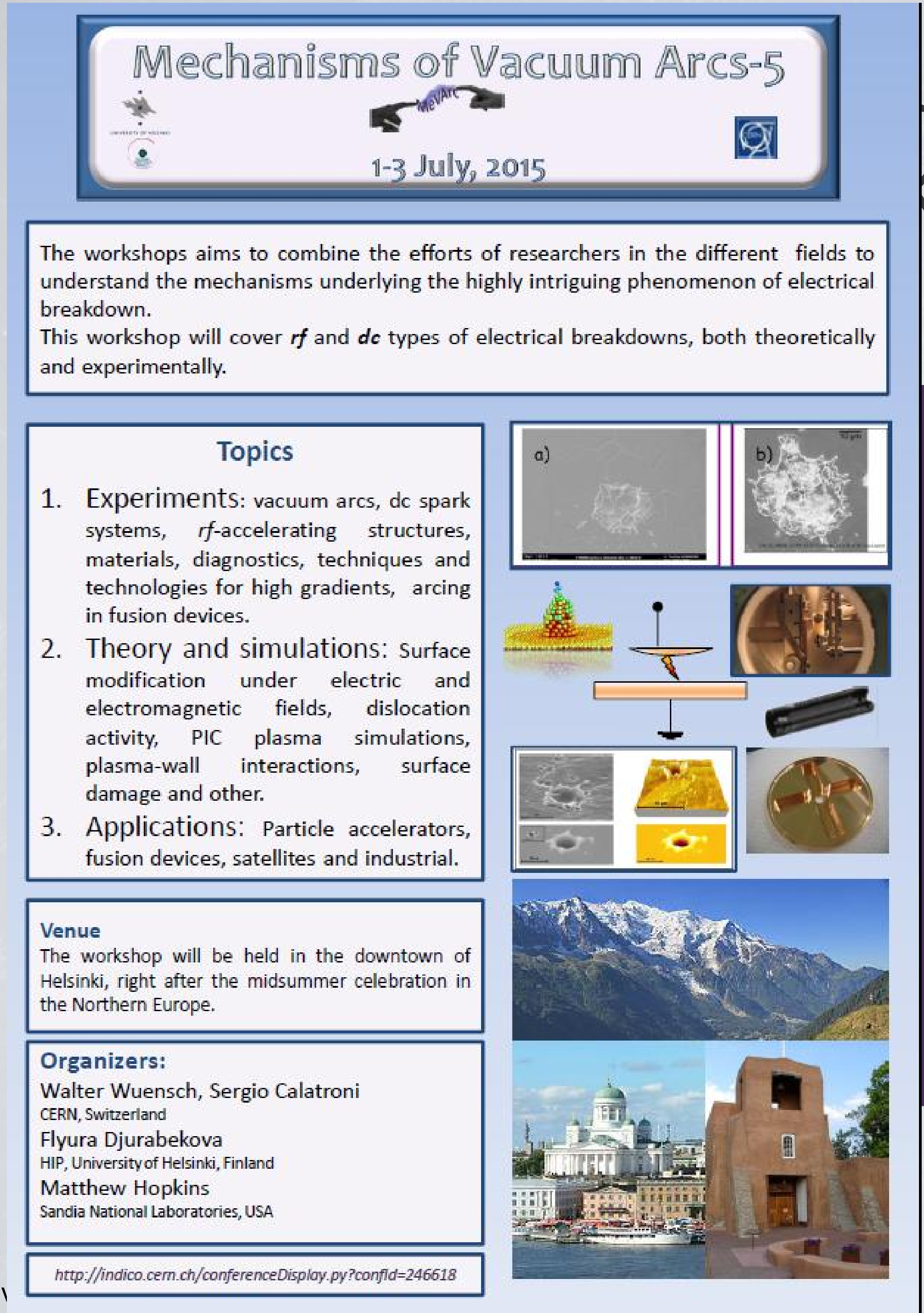
  - Hebrew university of Jerusalem
    - Dr. Yinon Ashkenazy

um arcs:

ki – Sandia



Mechanisms of Vacuum Arcs-5

1-3 July, 2015

The workshops aims to combine the efforts of researchers in the different fields to understand the mechanisms underlying the highly intriguing phenomenon of electrical breakdown.
This workshop will cover ***rf*** and ***dc*** types of electrical breakdowns, both theoretically and experimentally.

Topics

1. Experiments: vacuum arcs, dc spark systems, *rf*-accelerating structures, materials, diagnostics, techniques and technologies for high gradients, arcing in fusion devices.
2. Theory and simulations: Surface modification under electric and electromagnetic fields, dislocation activity, PIC plasma simulations, plasma-wall interactions, surface damage and other.
3. Applications: Particle accelerators, fusion devices, satellites and industrial.

Venue
The workshop will be held in the downtown of Helsinki, right after the midsummer celebration in the Northern Europe.

Organizers:
Walter Wuensch, Sergio Calatroni
CERN, Switzerland
Flyura Djurabekova
HIP, University of Helsinki, Finland
Matthew Hopkins
Sandia National Laboratories, USA

http://indico.cern.ch/conferenceDisplay.py?confId=246618

MeVARC–5
Helsinki
Finland
2015
1–3 July
(dates are subject to change)

Thank you for your attention!

Finland at midnight