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Atomistic approach in simulations of electrical breakdowns on metal surfaces

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Behind the model...

University of Helsinki, Finland

HIP


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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


M Sc Helga Timko
Plasma simulations
(CERN, Switzerland)


Dr Lotta Mether
Plasma simulations
CERN, Switzerland

Inspiration comes from CERN, Geneva


Dr. Walter Wuensch

Sergio Calatroni

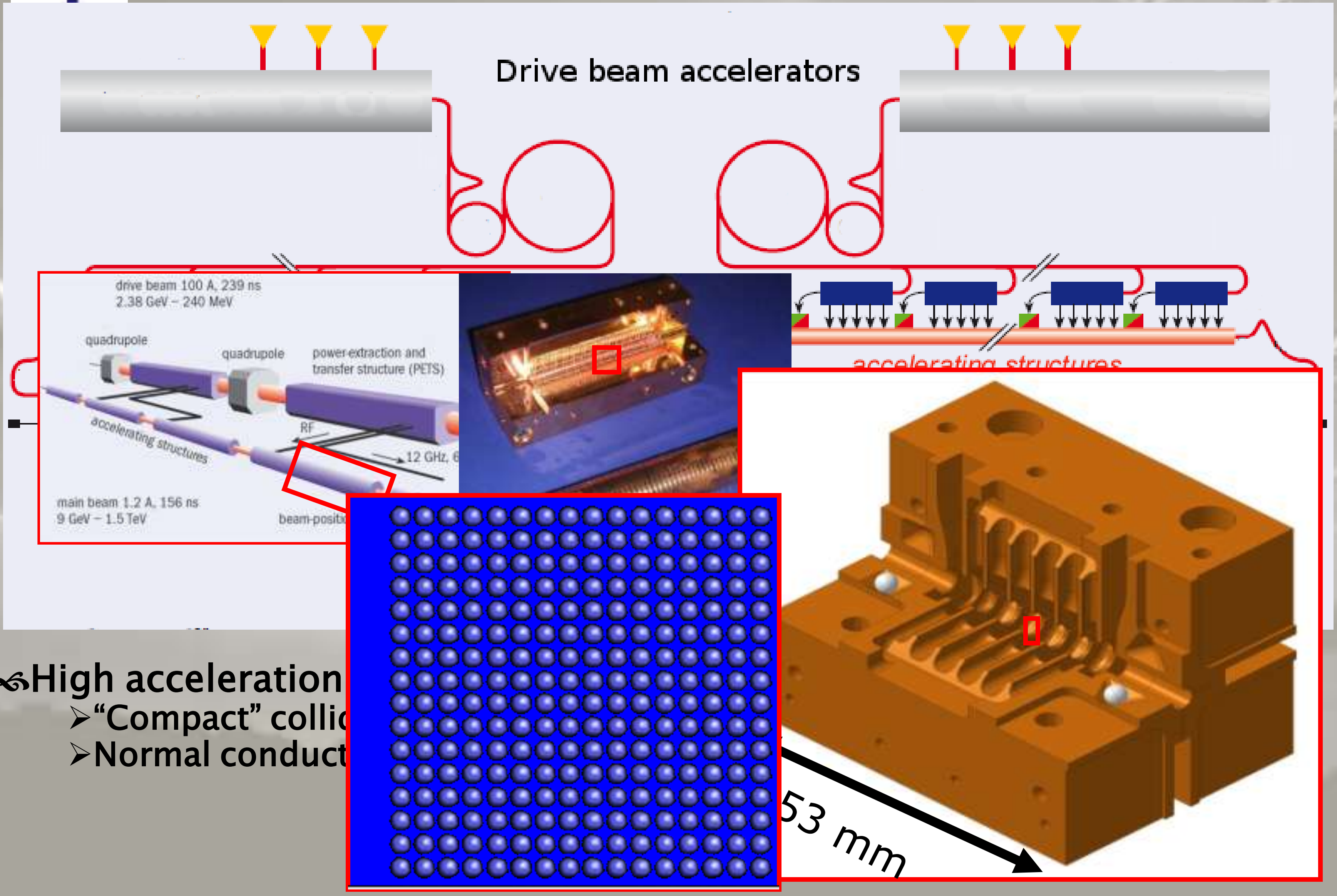
Outline

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


Accelerator Laborary, Helsinki


CERN, Geneva

CLIC: "Compact" Linear Collider...



- High acceleration
  - "Compact" collic
  - Normal conduct

Multiscale model to simulate electrical breakdown

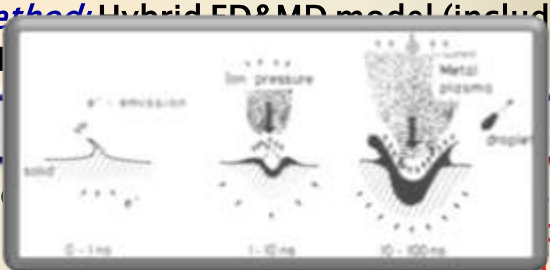
R. Behrisch, Plenum, 1986

~ sec/min

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
Lap



~few ns

~ sec/hours

Stage 3a: Onset of tip gr
Dislocation mechanism
Method: MD, Molecular Statics…

b: Evolution of surface
ology due to the given charge
distribution
Method: Kinetic Monte Carlo

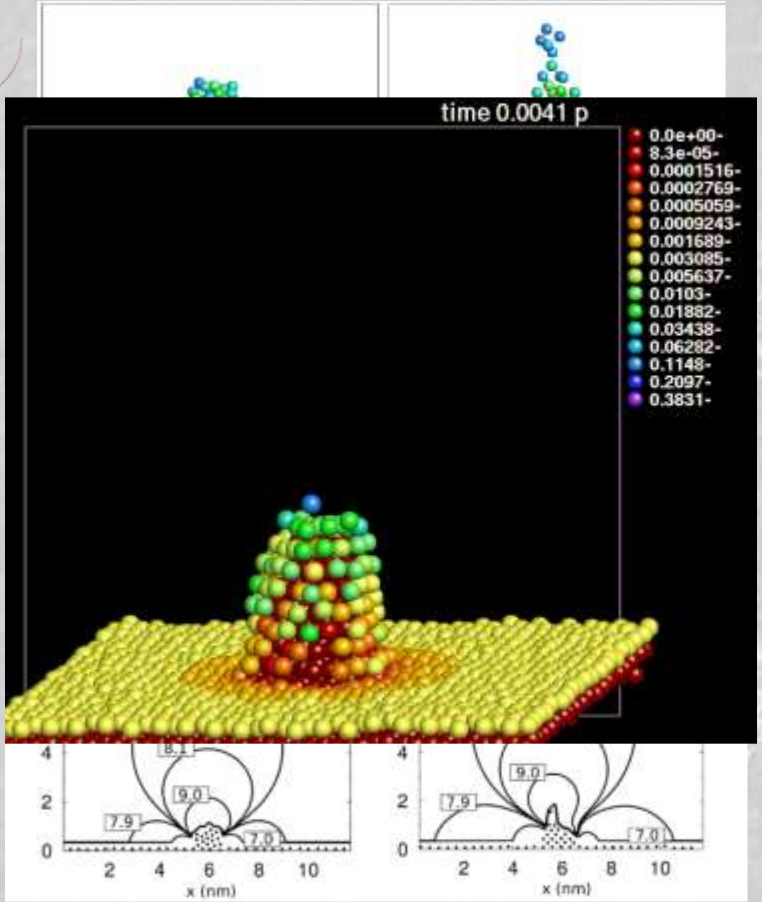
Stage 4: Plasma evolution, burning of arc
Method: Particle-in-Cell (PIC)

~10s ns

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

~100s ns

Evolution of a tip placed on Cu surface

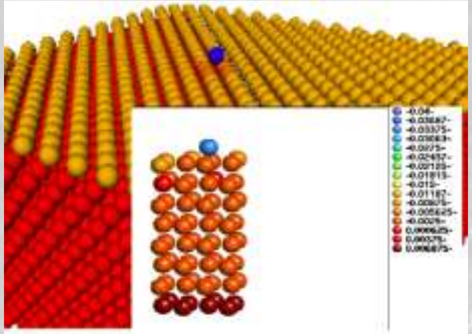


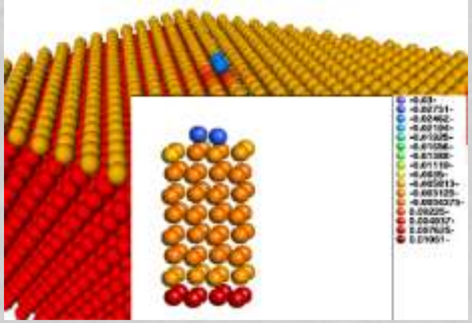
Details in F. Djurabekova, S. Parviainen, A. Pohjonen and K. Nordlund, PRE 83, 026704 (2011).

- We developed a novel approach 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.

DFT calculations to validate the charges on surface atoms

$E_0 = -1$ GV/m





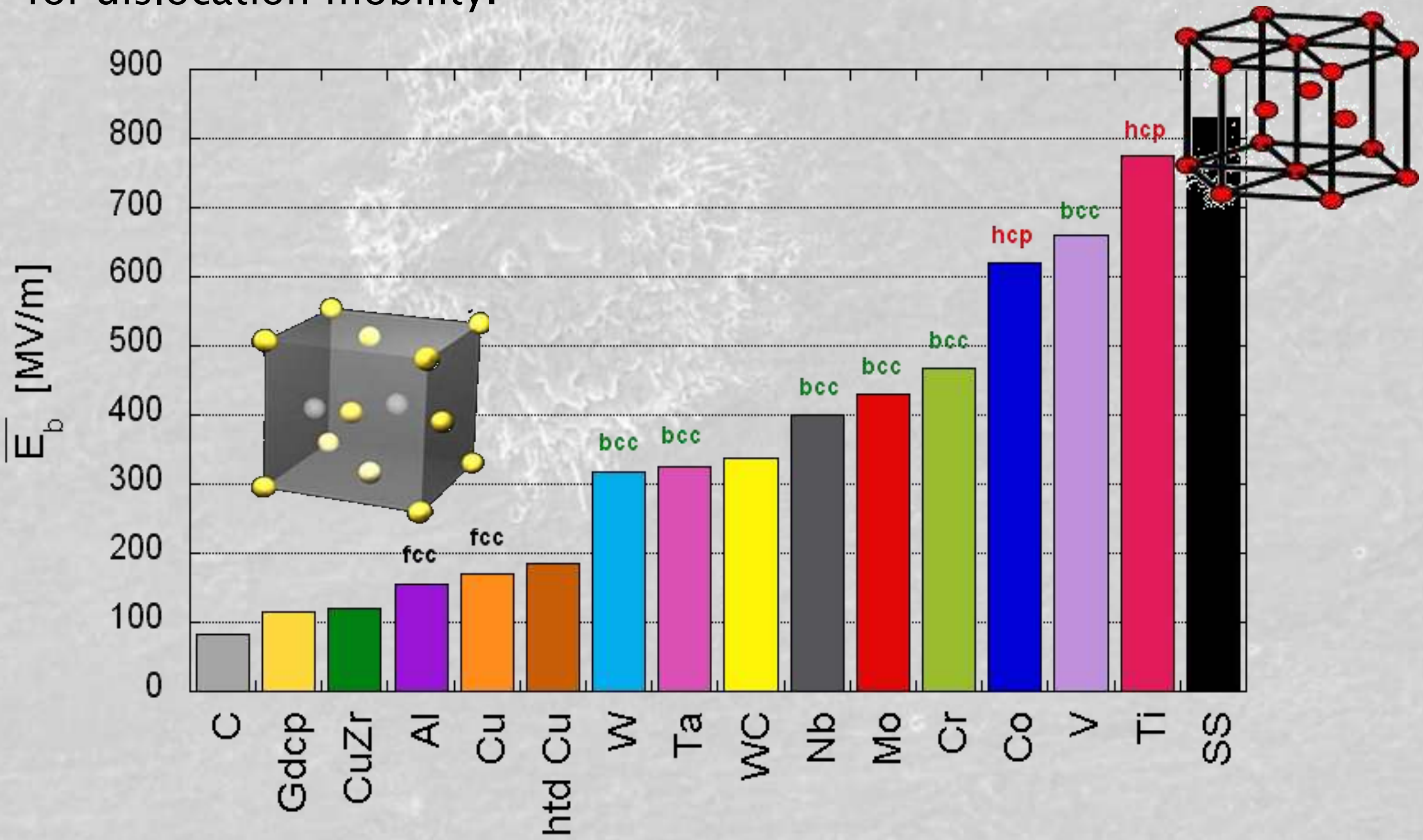
- DFT details:
  - Code: SIESTA
  - For exchange and correlations functionals the Perdew, Burke and Ernzerhof scheme of Generalized gradient approximation (GGA)
  - Slab organized in 8 layers+ 8 layers of vacuum
  - External field is added to calculate the electrostatic potential in the vacuum

$$\sigma = \varepsilon_0 \vec{E} = 5.53\times10^{16}\,\frac{\bar{e}}{m^2} \Leftrightarrow \sigma = \frac{Q_{surf}}{A_{surf}} = 5.49\times10^{16}\,\frac{\bar{e}}{m^2}$$

	An adatom		Double adatom	
	DFT, SIESTA	ED&MD	DFT, SIESTA	ED&MD
Charge (q_e) per adatom	−0.032	−0.0215	−0.025	−0.0177

Motivations: why we look for dislocations?

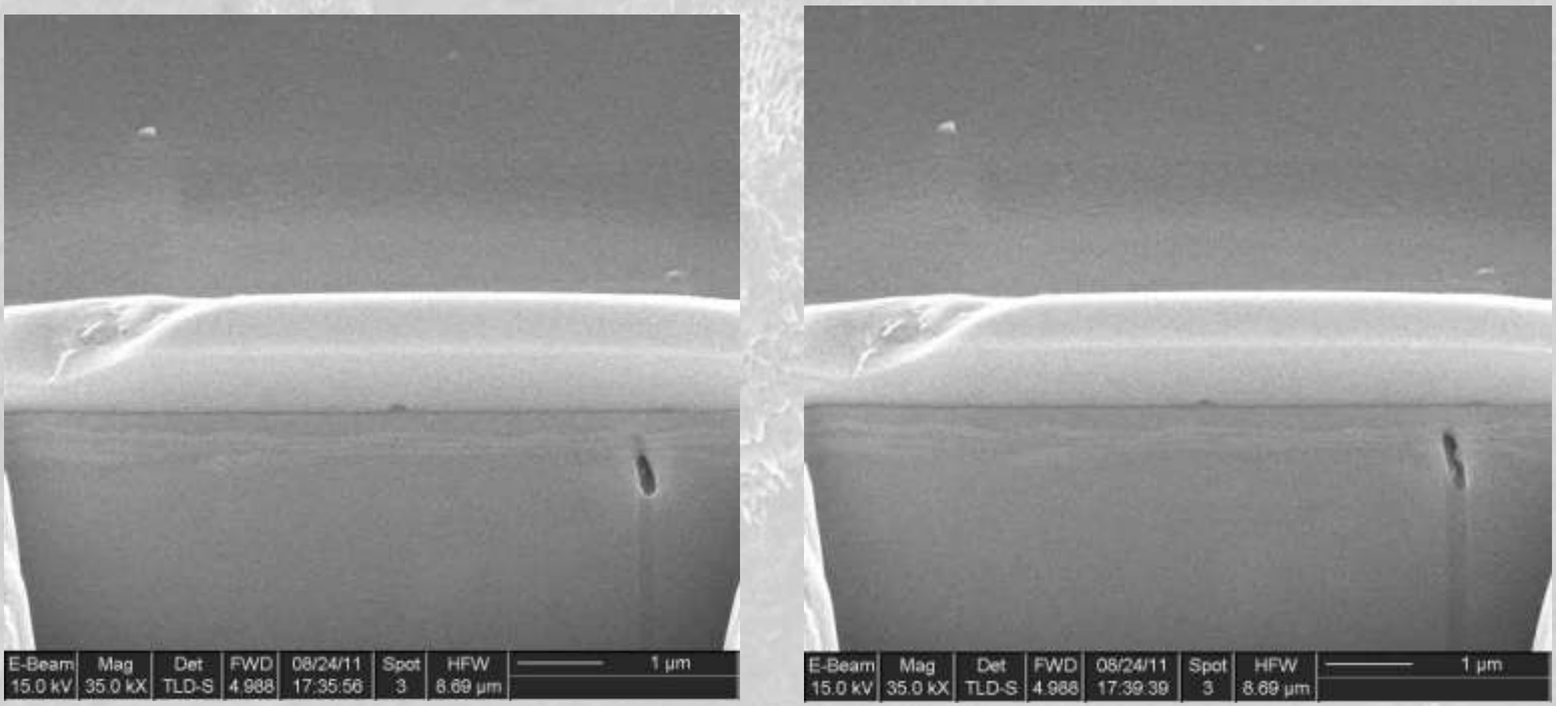
- The dislocation motion is strongly bound to the atomic structure of metals. In FCC (face-centered cubic) the dislocation are the most mobile and HCP (hexagonal close-packed) are the hardest for dislocation mobility.



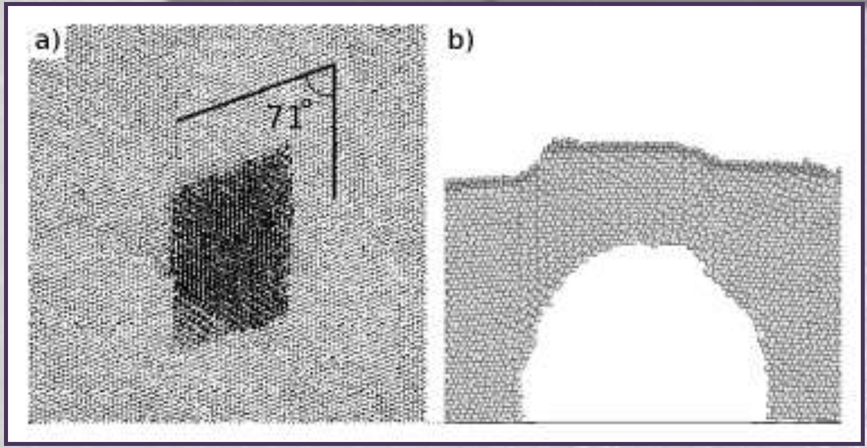
A. Descoeudres, F. Djurabekova, and K. Nordlund, DC Breakdown experiments with cobalt electrodes, CLIC-Note XXX, 1 (2010).

Experimental evidence of the voids

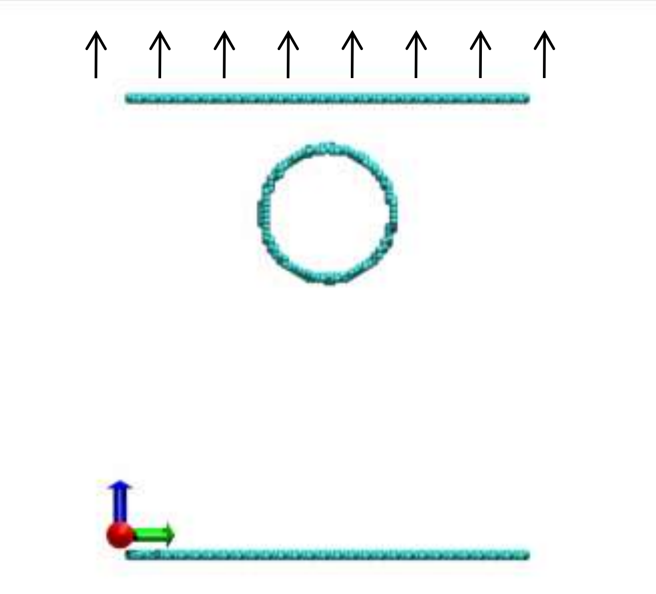
- SEM images by Dr. Tomoko Muranaka (Uppsala Univ.)

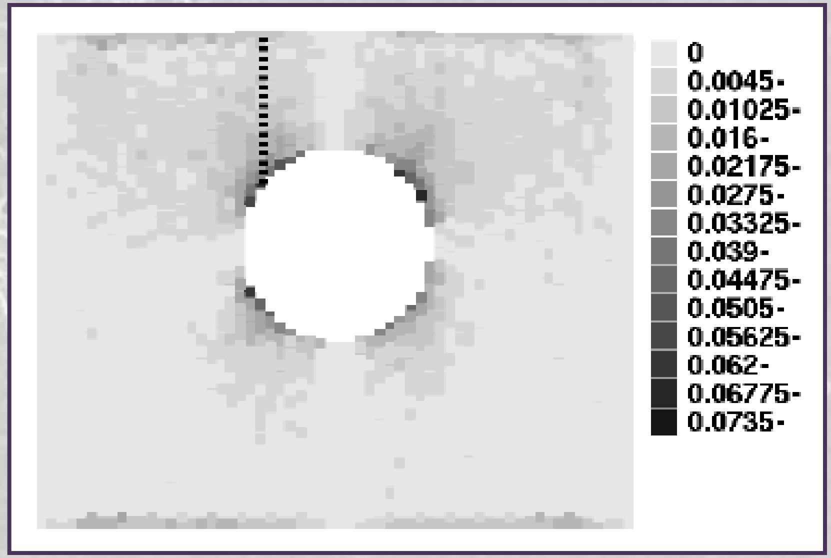


Voids: a lattice irregularity which can be a source of a protrusion growth



- 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.

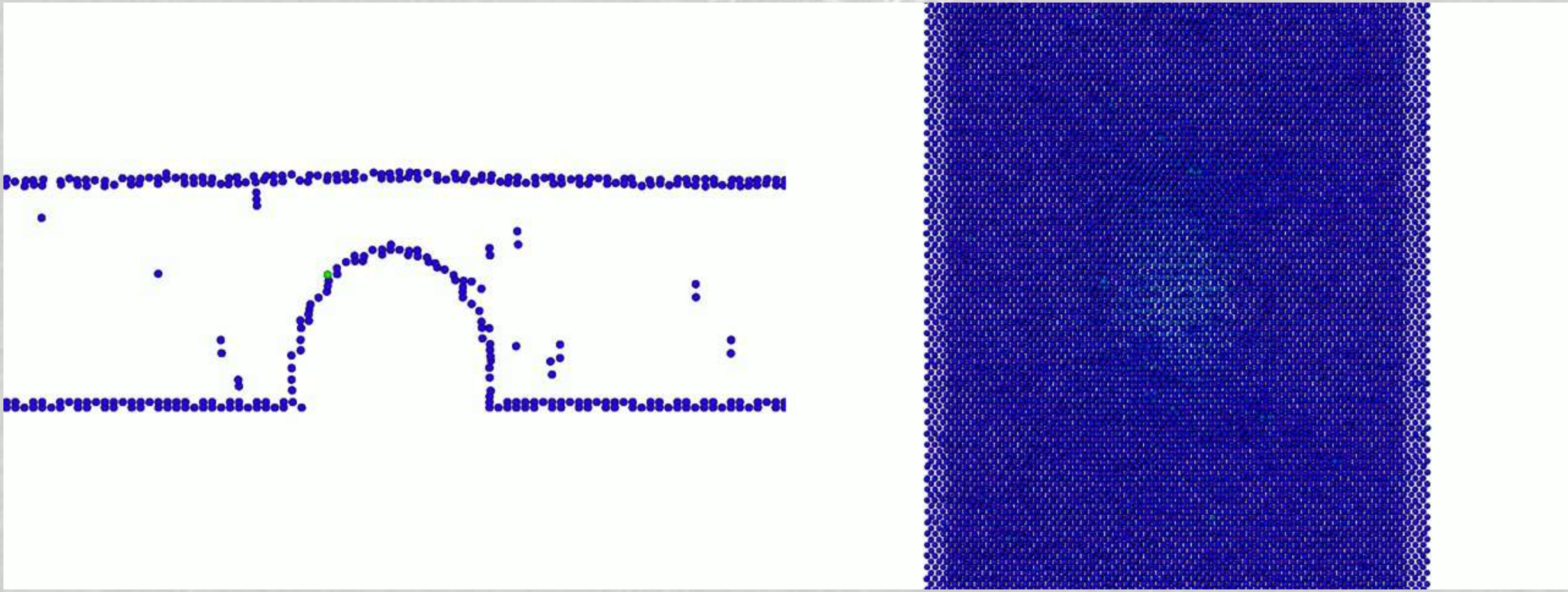




A. Pohjonen, F. Djurabekova, et al., Dislocation nucleation from near surface void under static tensile stress on surface in Cu, *Jour. Appl. Phys.* 110, 023509 (2011).

Concurrent ED-MD simulations of dislocations on a near-surface void

- Half-void of diameter 4nm in {110} Cu surface. (N of atoms≈ 170000 atoms…)
- E_0=22 GV/m (exaggeration is required to simulate the dislocation within the MD time span)
- T = 600 K

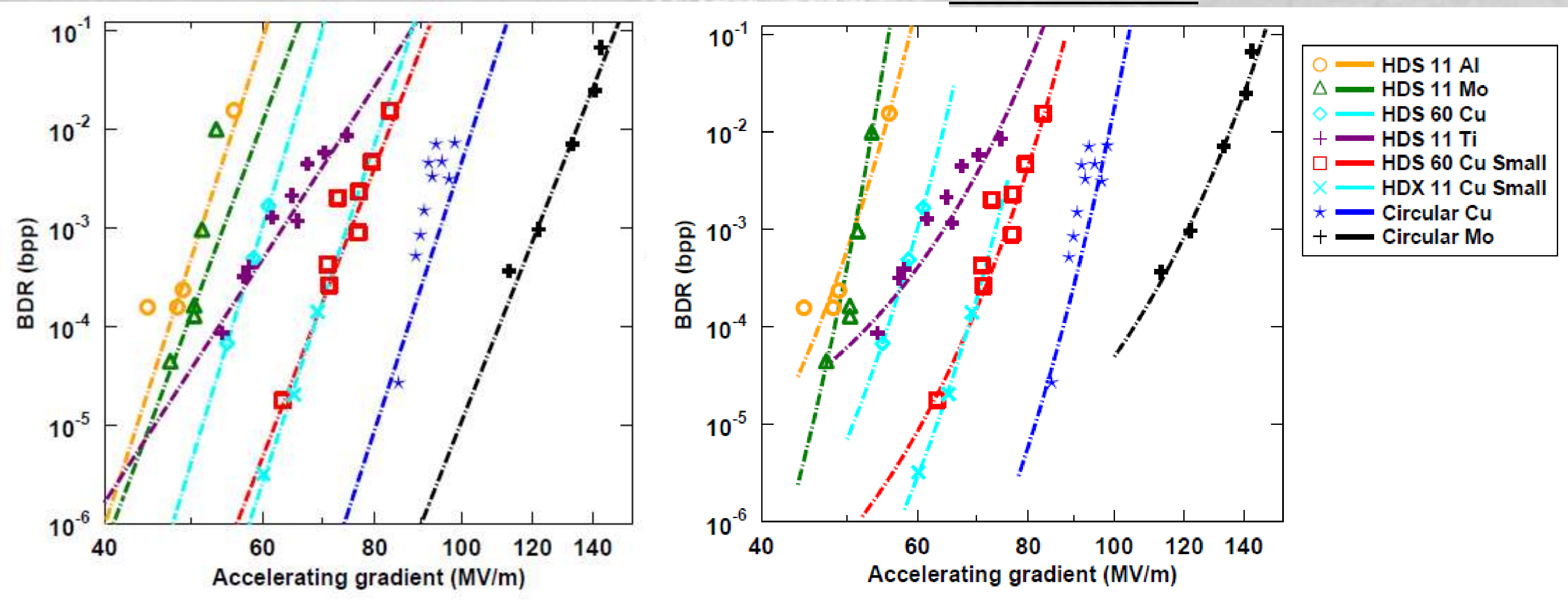


Dislocation-based model for electric field dependence

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

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

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

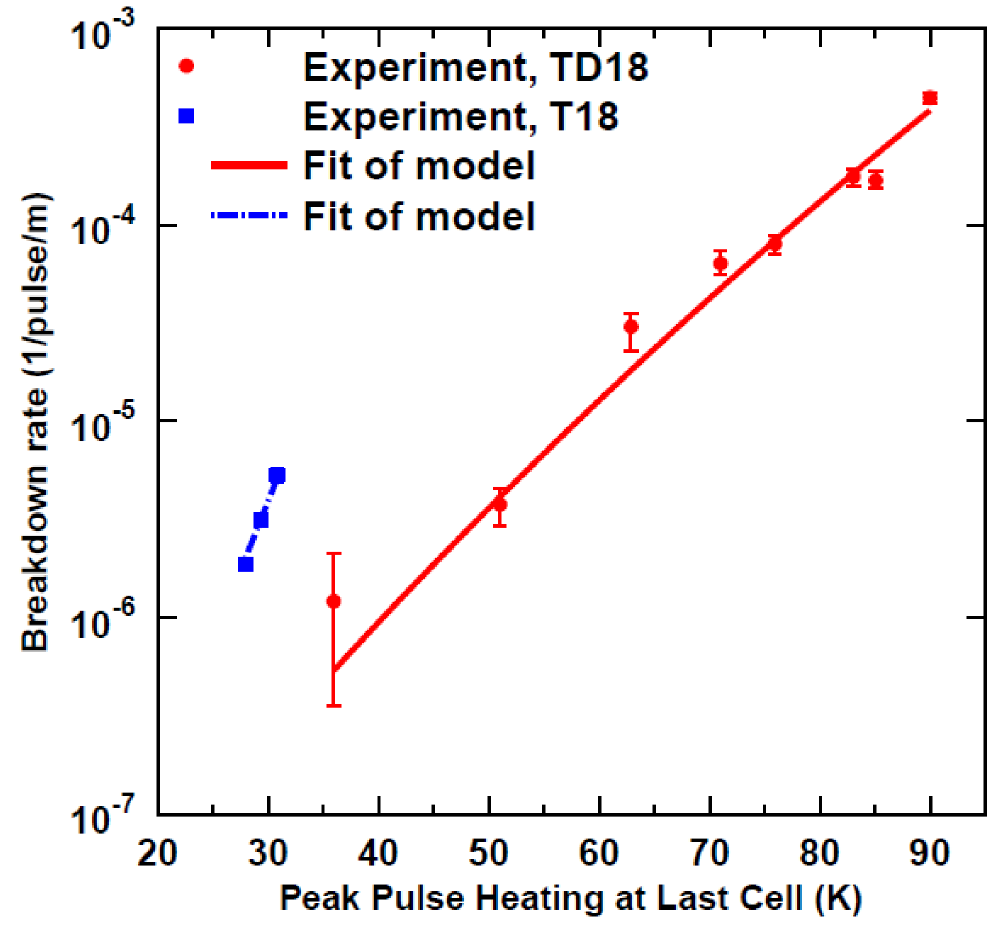


Power law fit

Stress model fit

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

Temperature dependence of BPP



- Experimental data on dependence of breakdown rate on the peak temperature increase in accelerating components

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

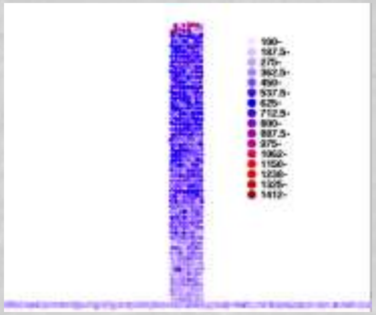
$$R_{BD} = a' c_0 \exp\left(\frac{-E^f + \varepsilon_0 E^2 \Delta V}{k_B (T_0 + \Delta T)} \right)$$

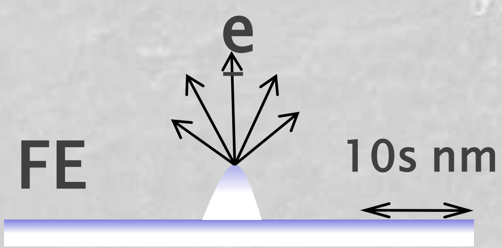
From tips to plasma: From FE to discharge currents

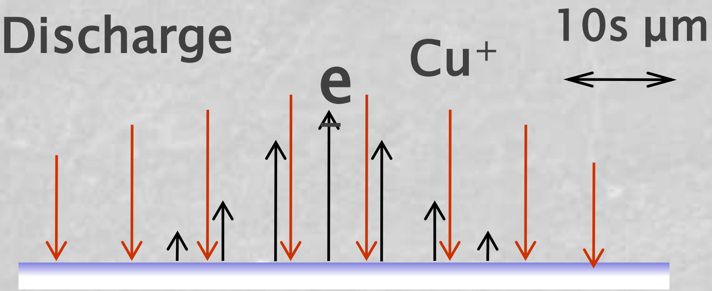
- In real life we can observe the full dynamic range of a vacuum discharge:
  - > 10s pA in ‘weak’ FE phase
  - Space charge limited ‘strong’ FE phase, typically ~ nA – µA
  - Discharge current, up to 10 – 100 A
- At the same time, the involved area changes:
  - Typically 10^{-20} – 10^{-14} m^2 for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

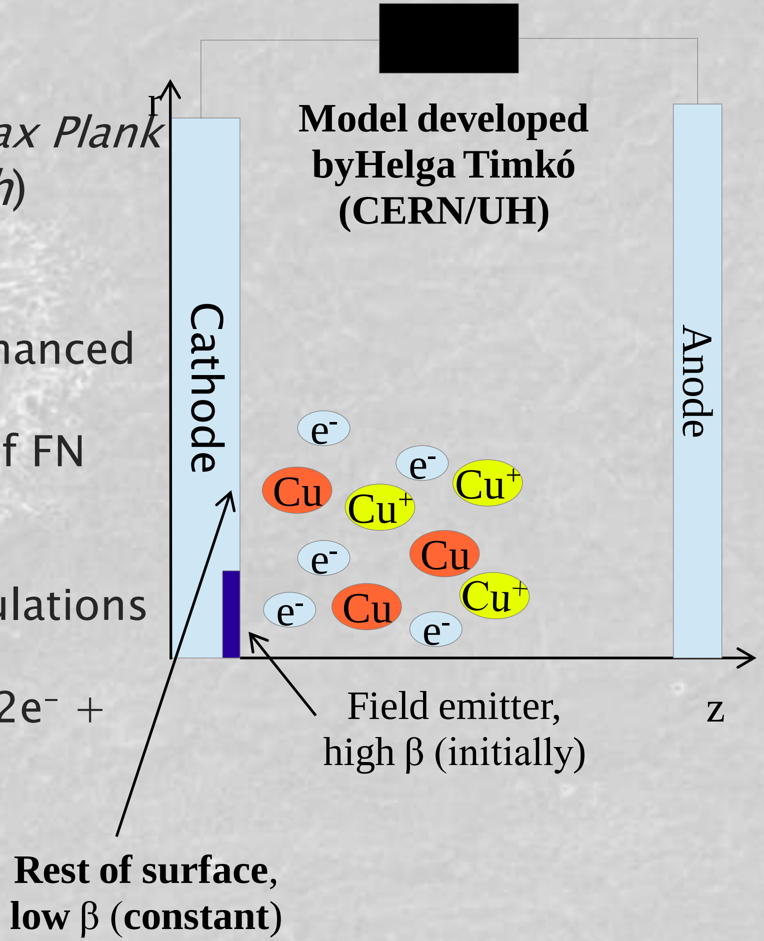






2D Arc-PIC in a nutshell

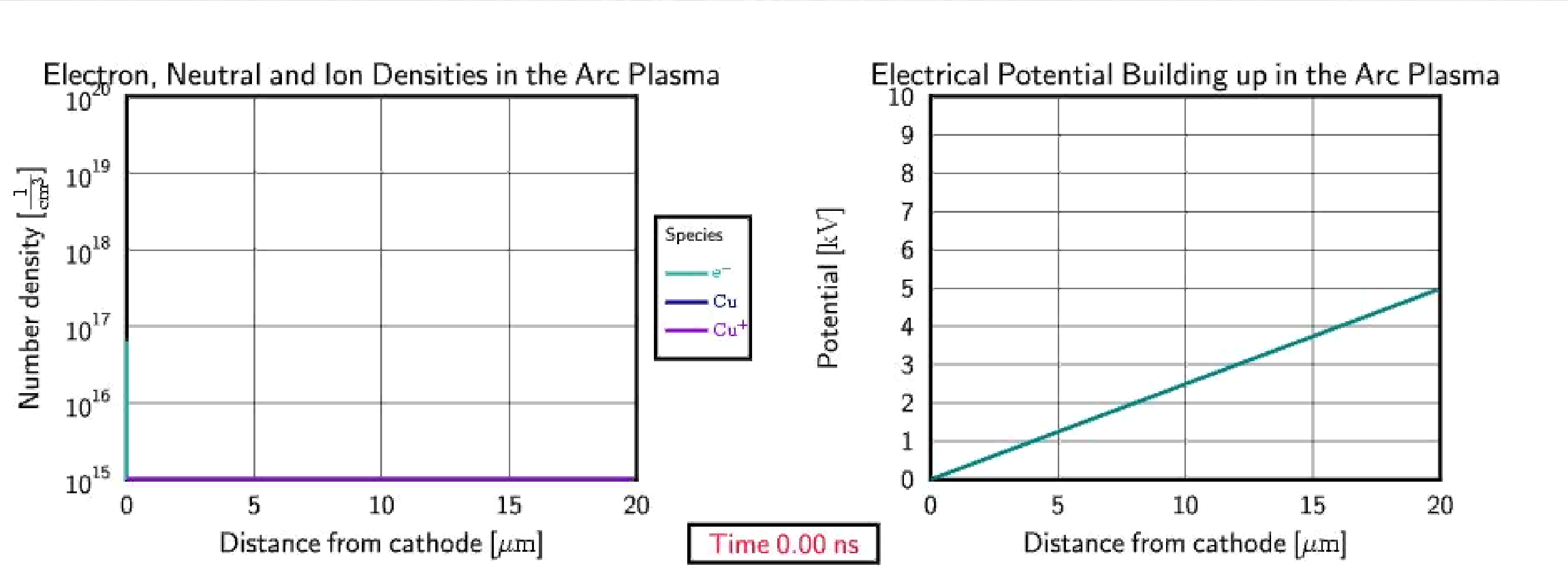
- 2d3v electrostatic PIC code with cylindrical symmetry
  - Particles: e^-, Cu, and Cu^+
  - Monte Carlo collision routines (*Max Plank Institute of Plasma Physics, K.Matyash*)
- Emission processes
  - Fowler-Nordheim field emission – enhanced by β
  - Simplified Cu evaporation – fraction of FN emission
  - 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)

Plasma build-up

Two conditions need to be fulfilled:

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



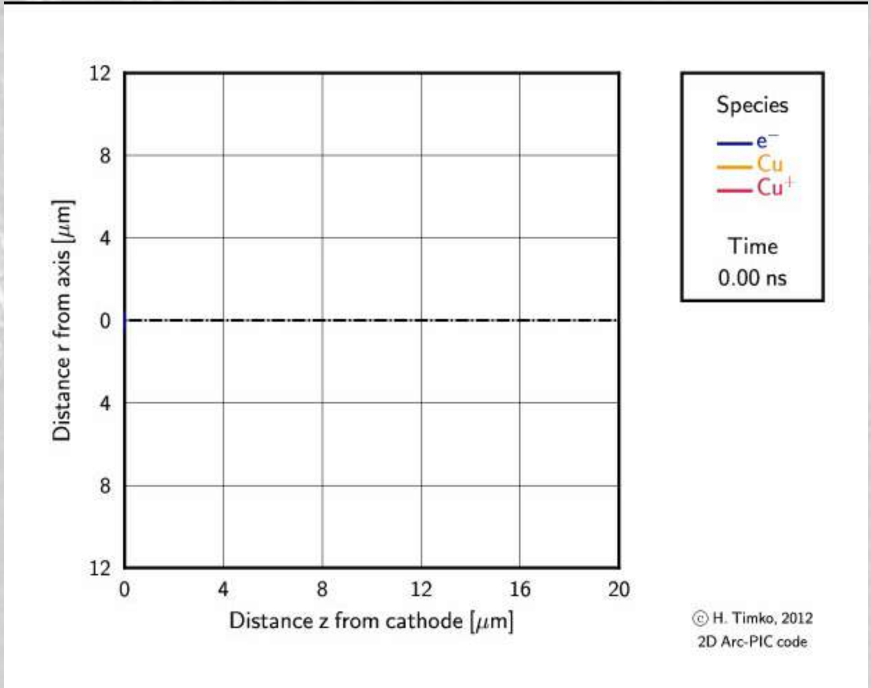
H. Timko, et al. A One-Dimensional Particle-in-Cell Model of Plasma Build-up in Vacuum Arcs, Contrib. Plasma Physics 51, 5 (2011).

From field emission to developed arc

– a typical 2D Arc-PIC simulation

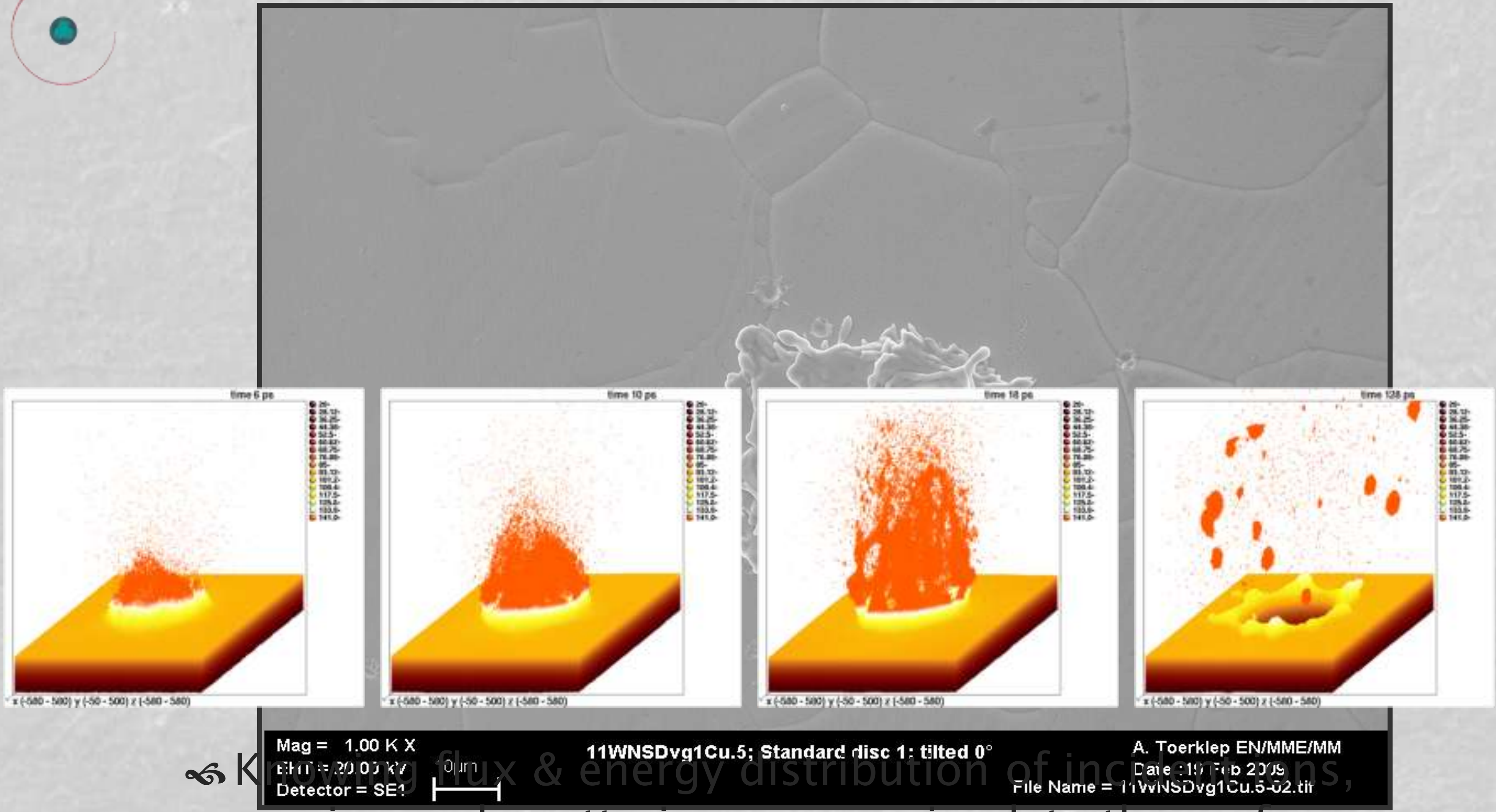
- Field emission + ionization
- Sudden ionization avalanche
- Sheath + quasi-neutral plasma forms
- Plasma self-maintaining if energy is available
- Neutrals fill entire gap

$\beta_0 = 35$, $\beta_f = 2$ Grid 240 × 400
$E_{ext} = 290$ MV/m $C_{ext} = 1$ nF
$r_{Cu/e} = 0.015$ $R_{em} = 0.4$ μm



H. Timko, L. Mether et al., Modeling of cathode plasma initiation in copper vacuum arc discharges via particle-in-cell simulations, Physics of Plasmas to be published

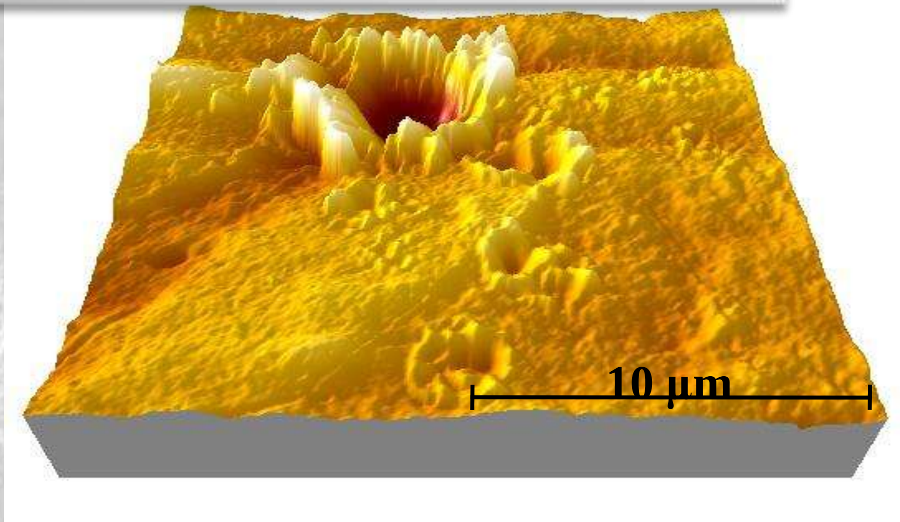
Cathode damage due to ion bombardment

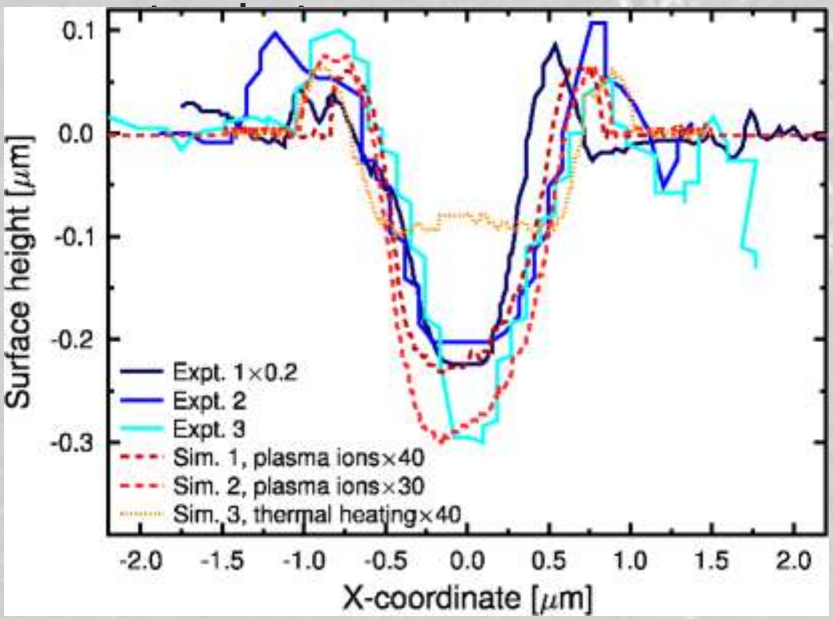


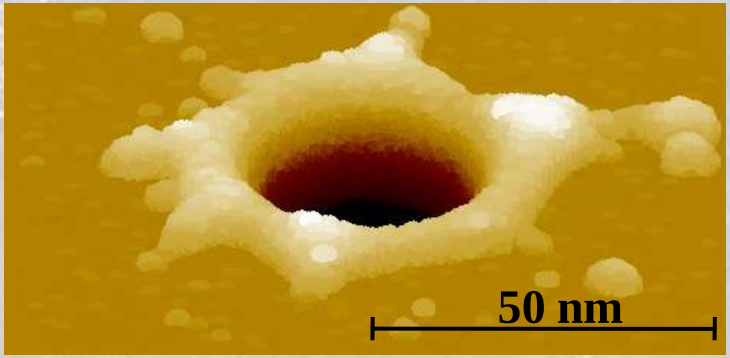
- Knowing flux & energy distribution of incident ions, erosion and sputtering we can simulate the surface damage with MD

Comparison to experiment

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







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

- We develop a multiscale model, which comprises the different physical processes (nature and time wise) probable right before, during and after an electrical breakdown event:
  - All the parts of the general model are pursued in parallel. We develop intense activities to cover all possible aspects.
- Our modeling shows:
  - Plasma is fed from the tips grown under the high electric field
  - Tip growth can be explained by the relaxation of stresses inside of a material by the dislocation motion
  - A dislocation-mediated mechanism can explain the high slopes of breakdown rates against the accelerating fields

MeVARC2012

Mechanisms of Vacuum Arcs
Albuquerque, New-Mexico, USA
2-4 October

Thank you!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N COLLISON
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A GLUONE DECECTION COLLISION
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