# Computer simulations of Cu surface behavior before and after a breakdown event

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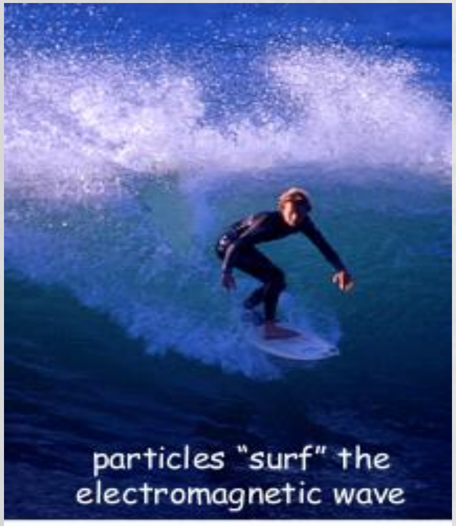
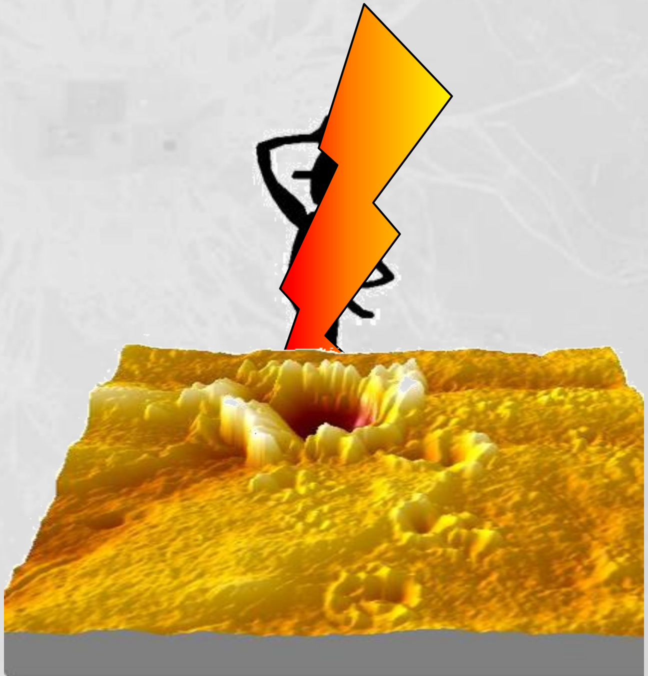
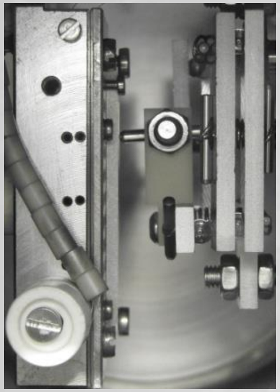
# Outline

- Our vision of processes preceding a breakdown event
  - Multiscale/multiphysics modeling
- Work function of different faces of Cu polycrystallites
- Voids under the surface: a possible source of protrusions
- What happens to the surface after the impact?

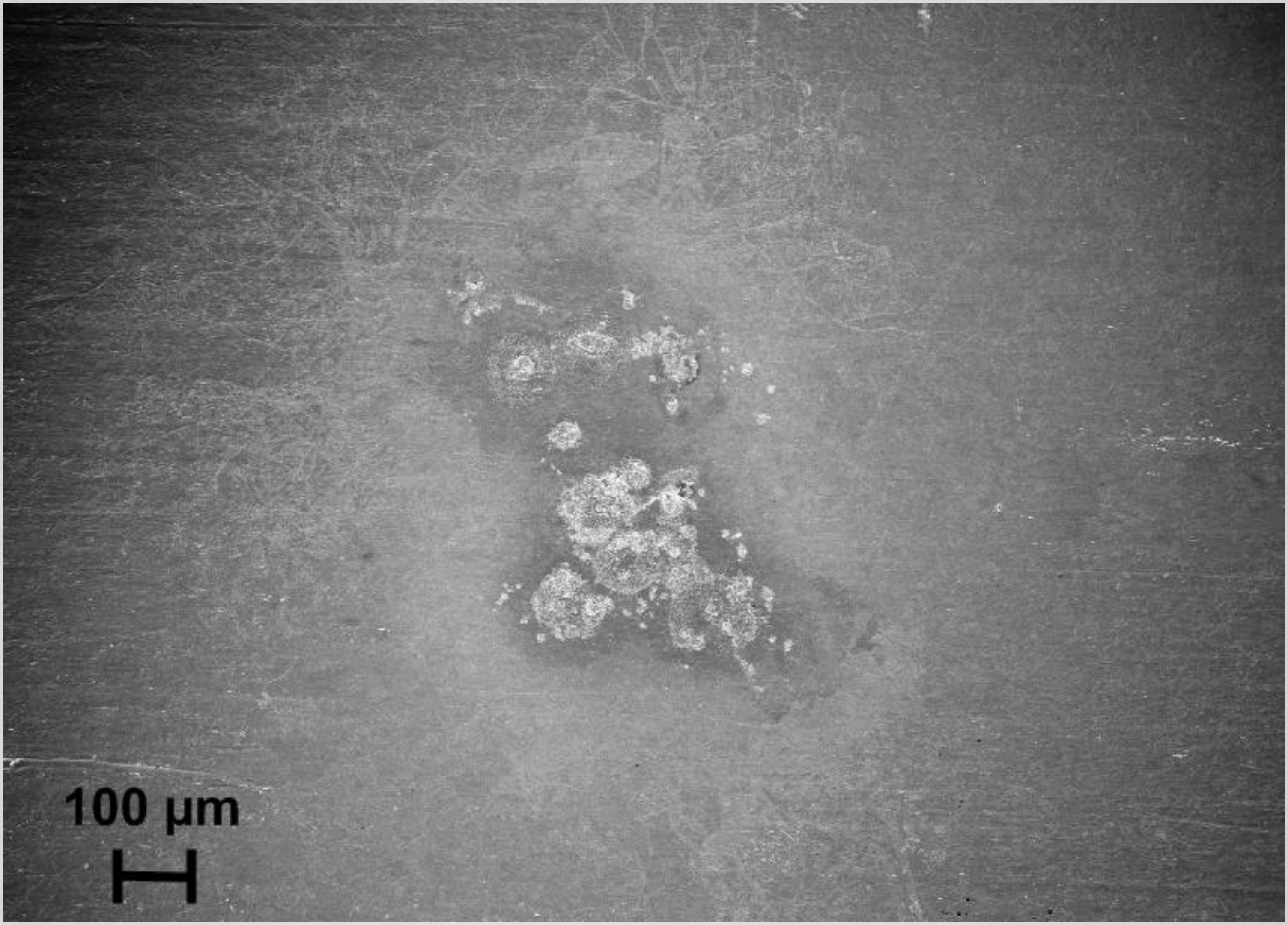


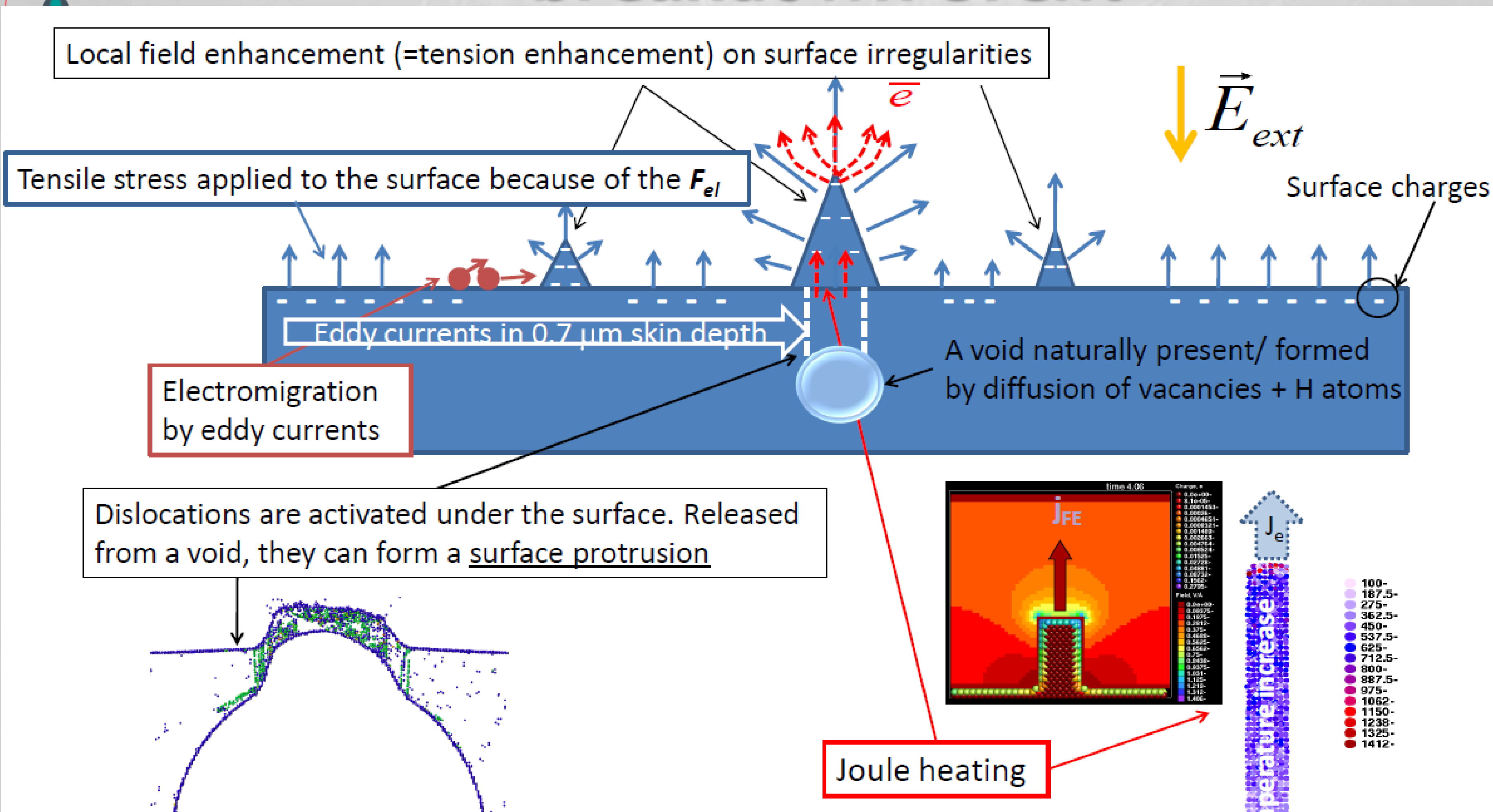
# Problem at hand



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

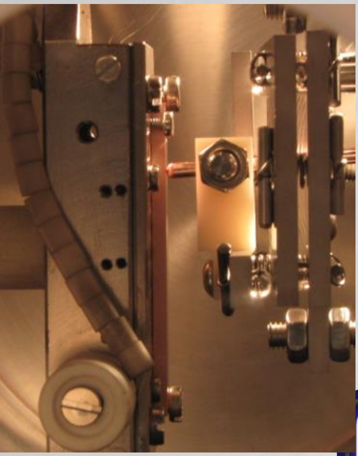


# Our vision of processes prior to breakdown event




Schematic of processes under high electric field

# … Multiscale/multiphysics computational model



**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 (V.Jansson)

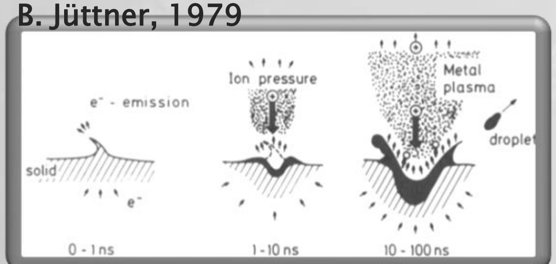
**Stage 4:** Plasma evolution, burning of arc
*Method:* Particle-in-Cell (PIC) (CERN)

~10s ns

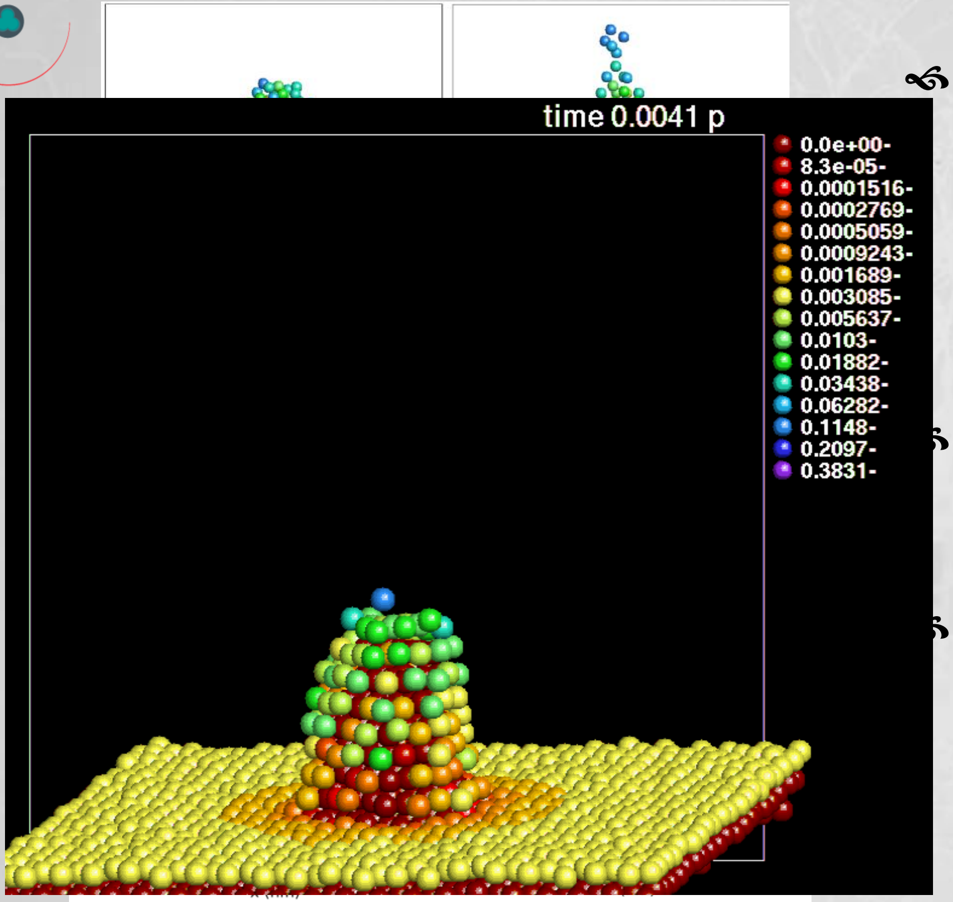
**Stage 5:** Surface damage due to the intense ion bombardment from plasma
*Method:* Arc MD

~100s ns

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



# Evolution of a tip placed on Cu surface

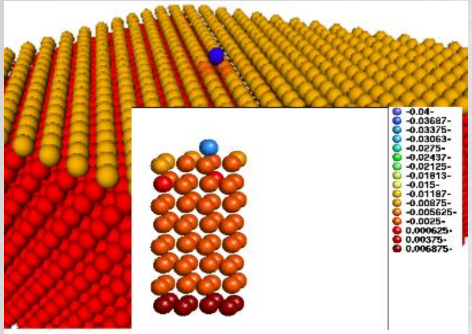


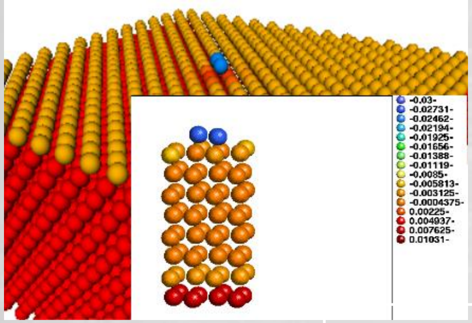

- We developed a novel approach to follow the dynamic evolution of partial charge on surface atoms by combining the MD and classical ED (solving Laplace equation)
- The dynamics of atom charges follows the shape of electric field distortion on tips on the surface
- Temperature on the surface tips is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

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

# DFT calculations to validate the charges on surface atoms

$E_o$=−1 GV/m

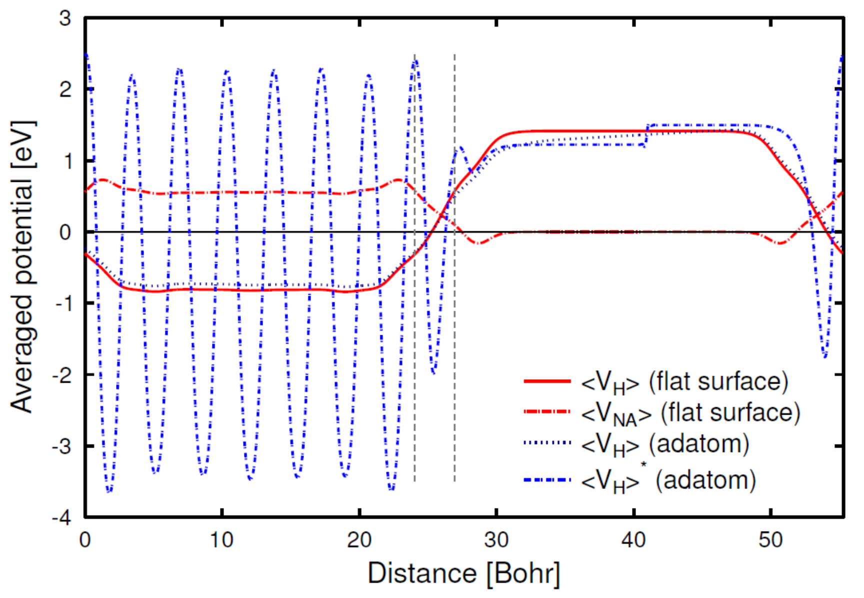




- DFT details:
  - Code: SIESTA
  - For exchange and correlations functionals the Perdew, Burke and Ernzerhof scheme of Generalized gradient approximation (GGA)
  - Slab organized in 8 layers+ 8 layers of vacuum
  - External field is added to calculate the electrostatic potential in the vacuum

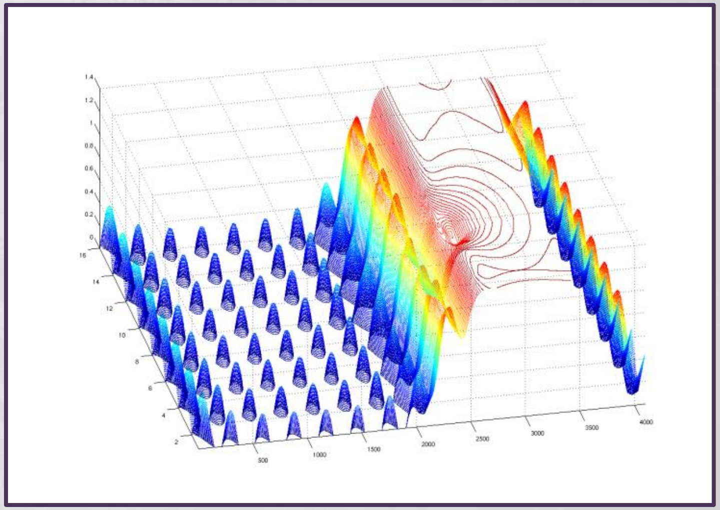
| | An adatom | | Double adatom | |
|---|---|---|---|---|
| | DFT, SIESTA | ED&MD | DFT, SIESTA | ED&MD |
| Charge ($q_e$) per adatom | −0.034 | −0.043 | −0.025 | −0.035 |

# Workfunction near an adatom in Cu




- We have calculated the workfunction for Cu surface when a single adatom is present

$$\Phi = -E_F + W_s + \Delta E_V$$

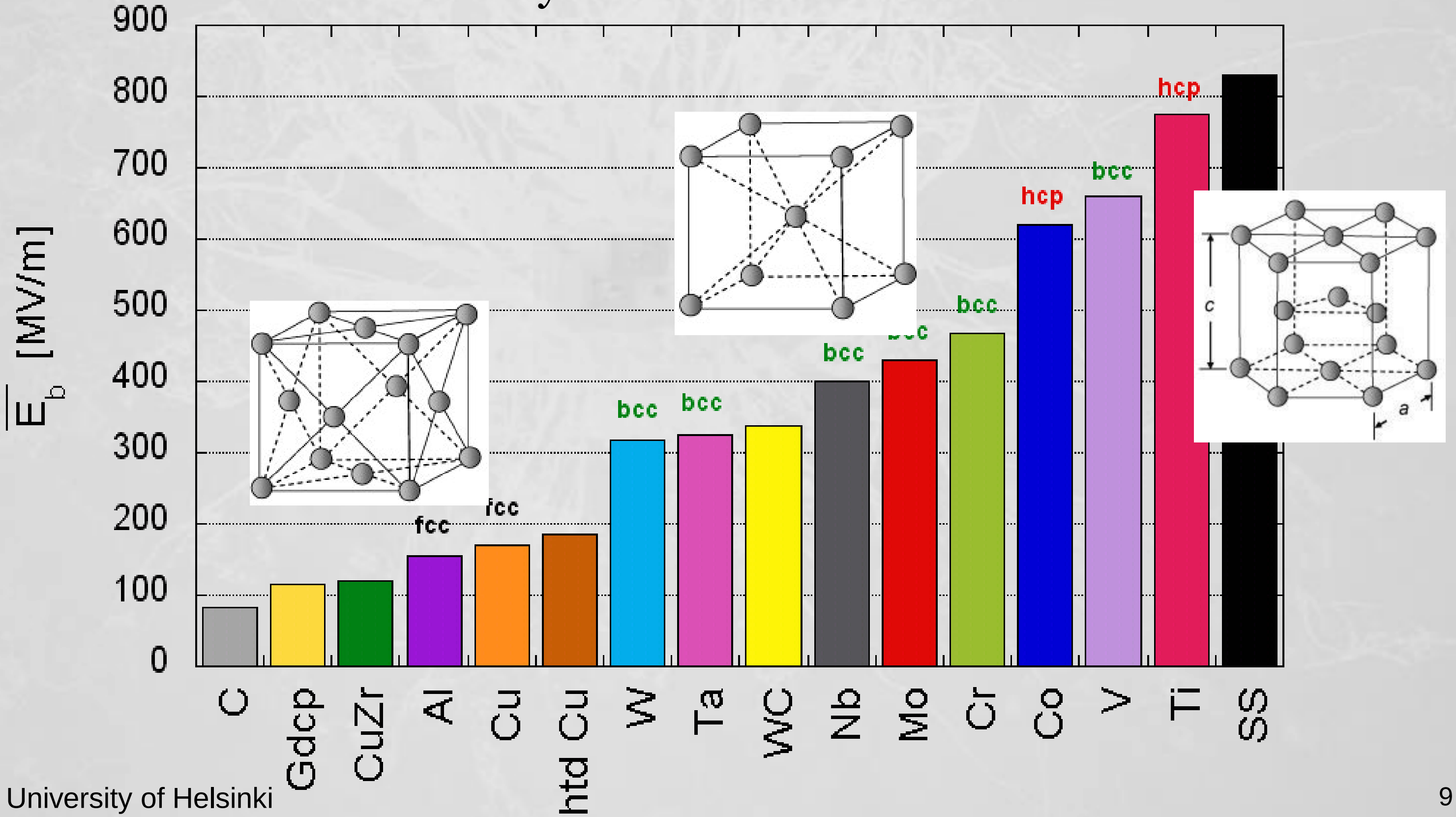


| | Cu(100) | Cu(110) | Cu(111) |
|---|---|---|---|
| Φ (LDA) | 4.898 | 4.708 | 5.170 |
| Φ (exp) | 4.599 | 4.490 | 4.980 |
| Φ (our) | 4.74 | 4.64 | 5.06 |

| | Cu(100) | Cu(110) | Cu(111) | Edge(100) |
|---|---|---|---|---|
| ΔΦ (with adatom), eV | -0.28 | -0.1 | -0.54 | -0.15 |

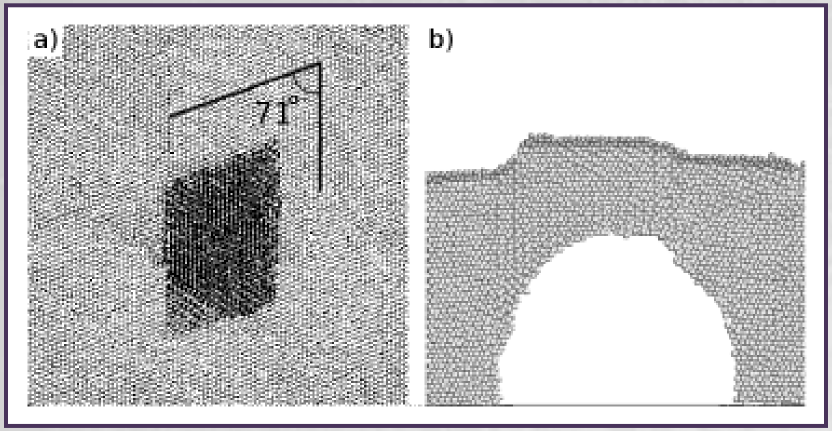
# What are the field emitters?
# Why do we look for dislocations?

- 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.

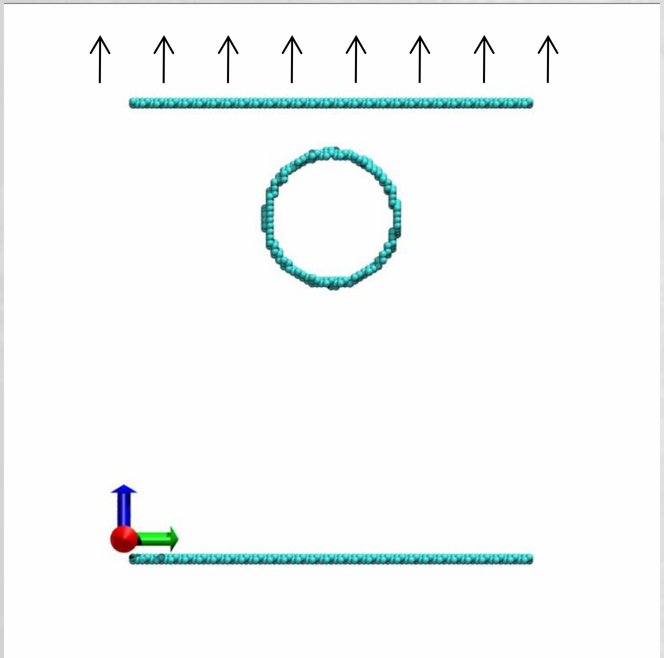


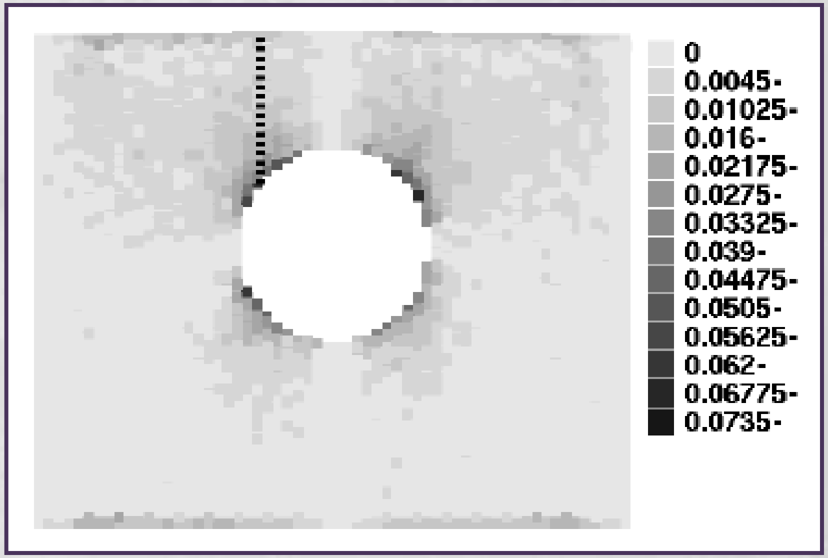

**A. Descoeudres, F. Djurabekova, and K. Nordlund, DC Breakdown experiments with cobalt electrodes, CLIC-Note XXX, 1 (2010).**

# A void hypothesis as a lattice irregularity



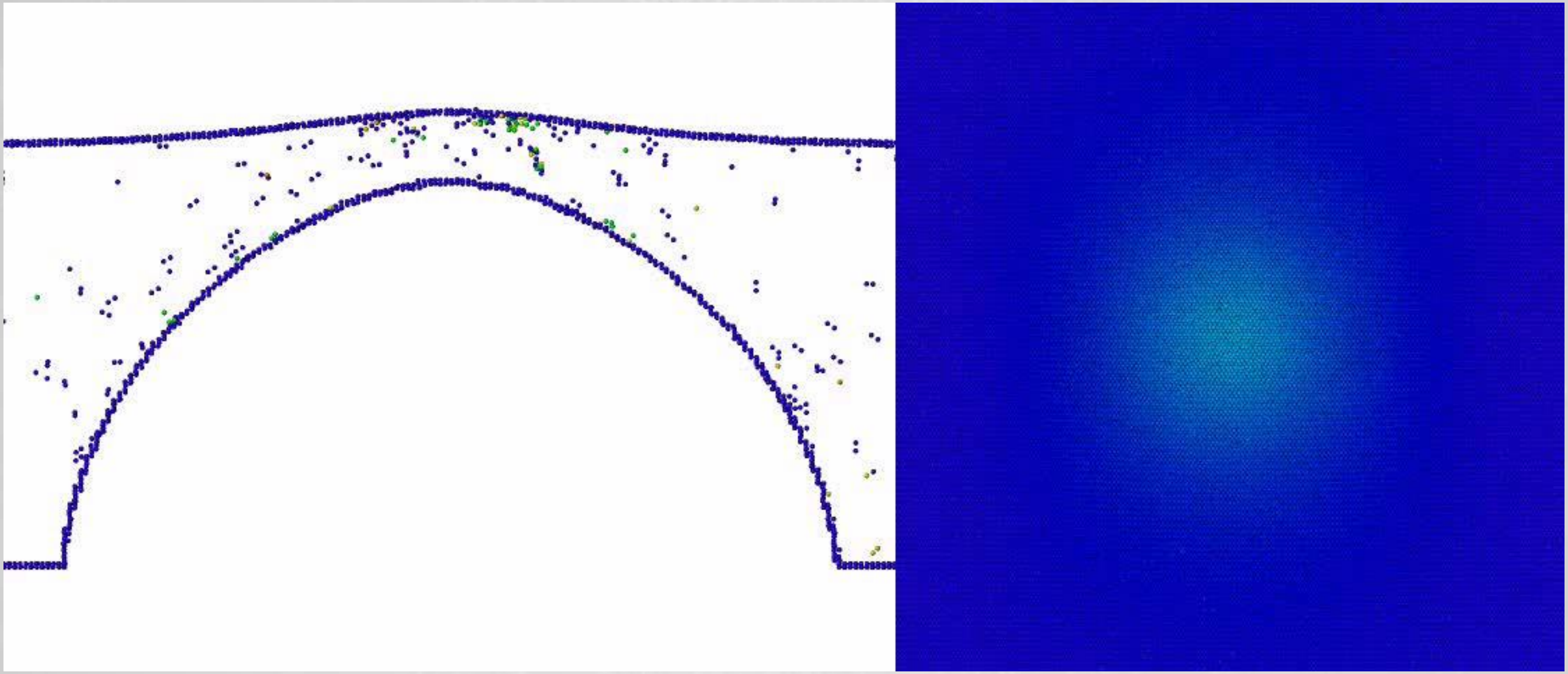

- We simulated a void near {110} Cu surface , when the high tensile stress is applied on the surface. Bottom is fixed, lateral boundary allowed to move in z direction.






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

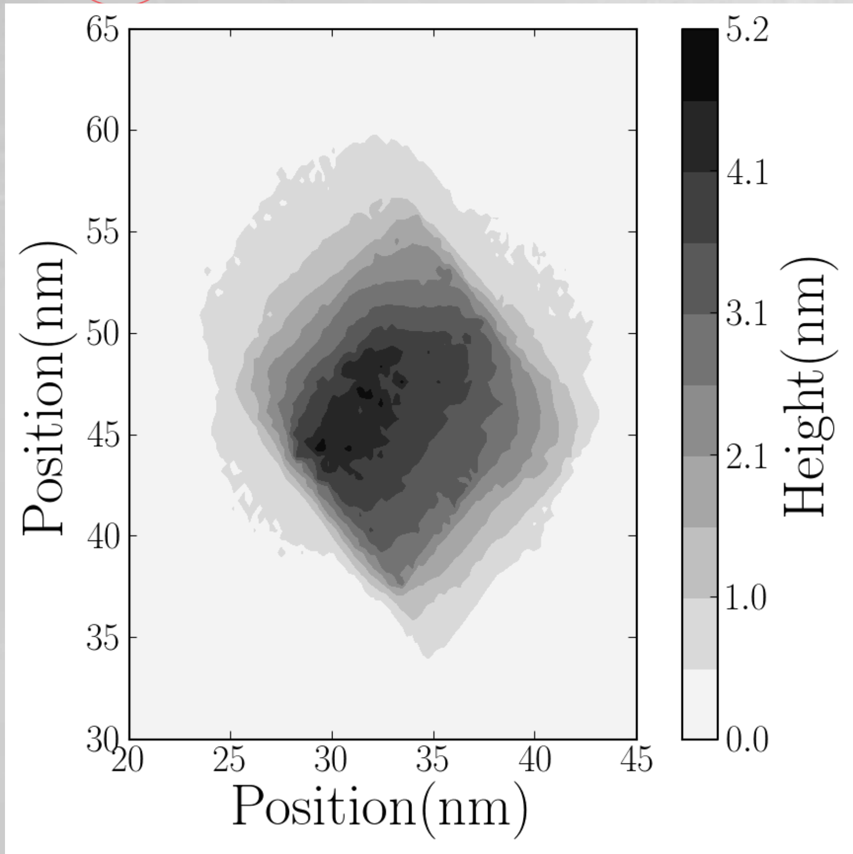
# Switching on the electric field above the surface

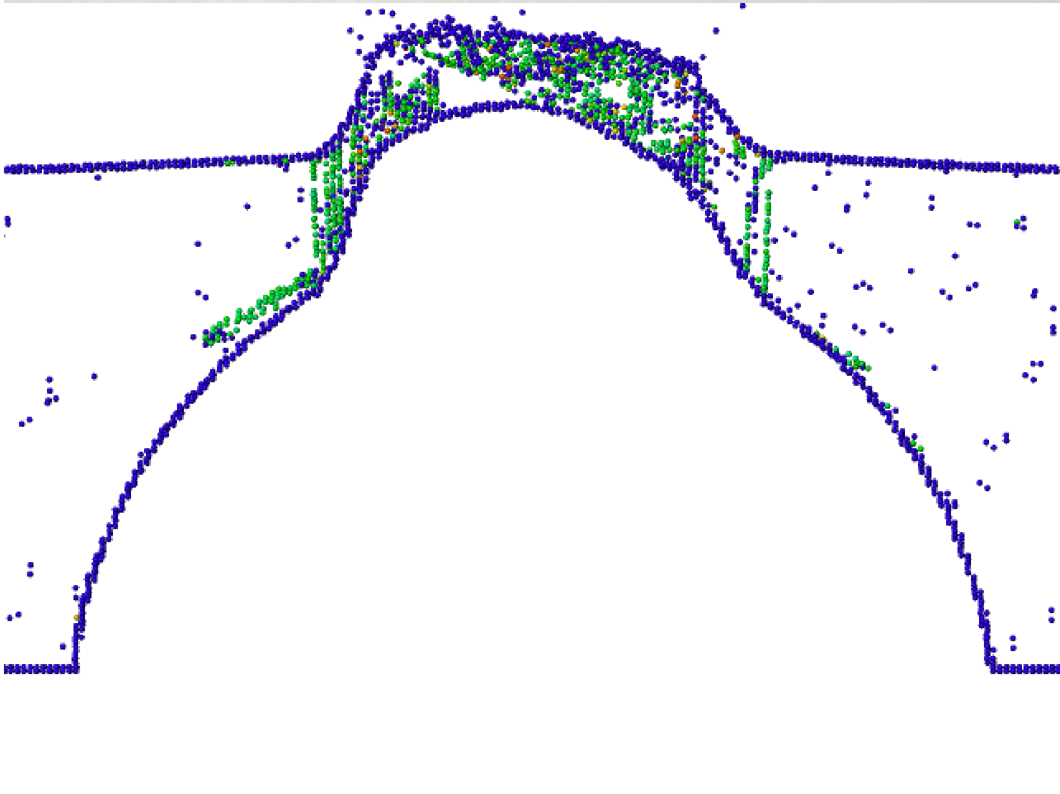


- We have now finished the analysis of the behavior of a void under tensile stress due to the electric field (Simulations now done with the hybrid ED-MD code, where the electric field effect is accounted explicitly)

**[A. S. Pohjonen, S. Parviainen, T. Muranaka, and F. Djurabekova, Journal of Appl. Physics 114, 033519 (2013)]**

# "Catastrophic"growth of a protrusion at the void

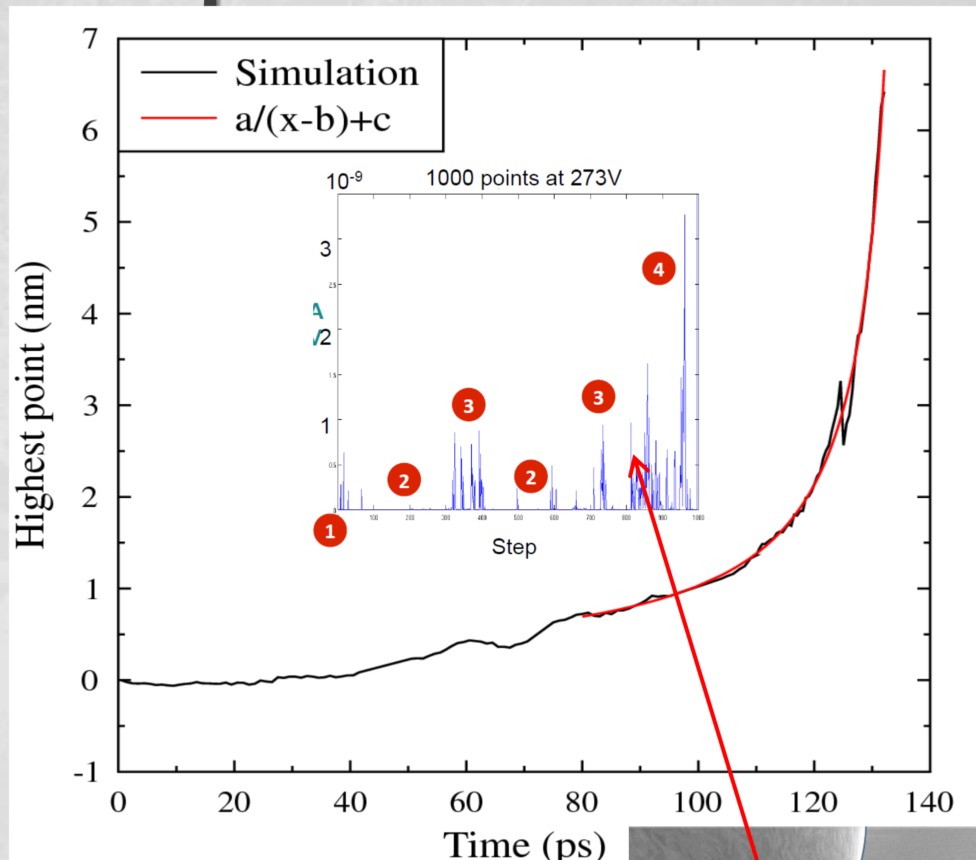


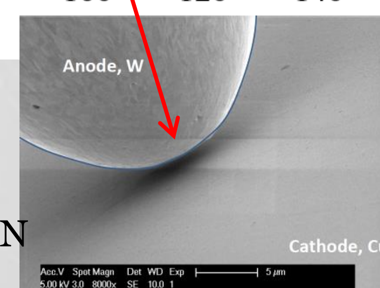



- . the top view and a slice of the system at time t = 130 ps when the fully developed protrusion is clearly visible.

# The "catastrophic" growth of a protrusion in the presence of the field

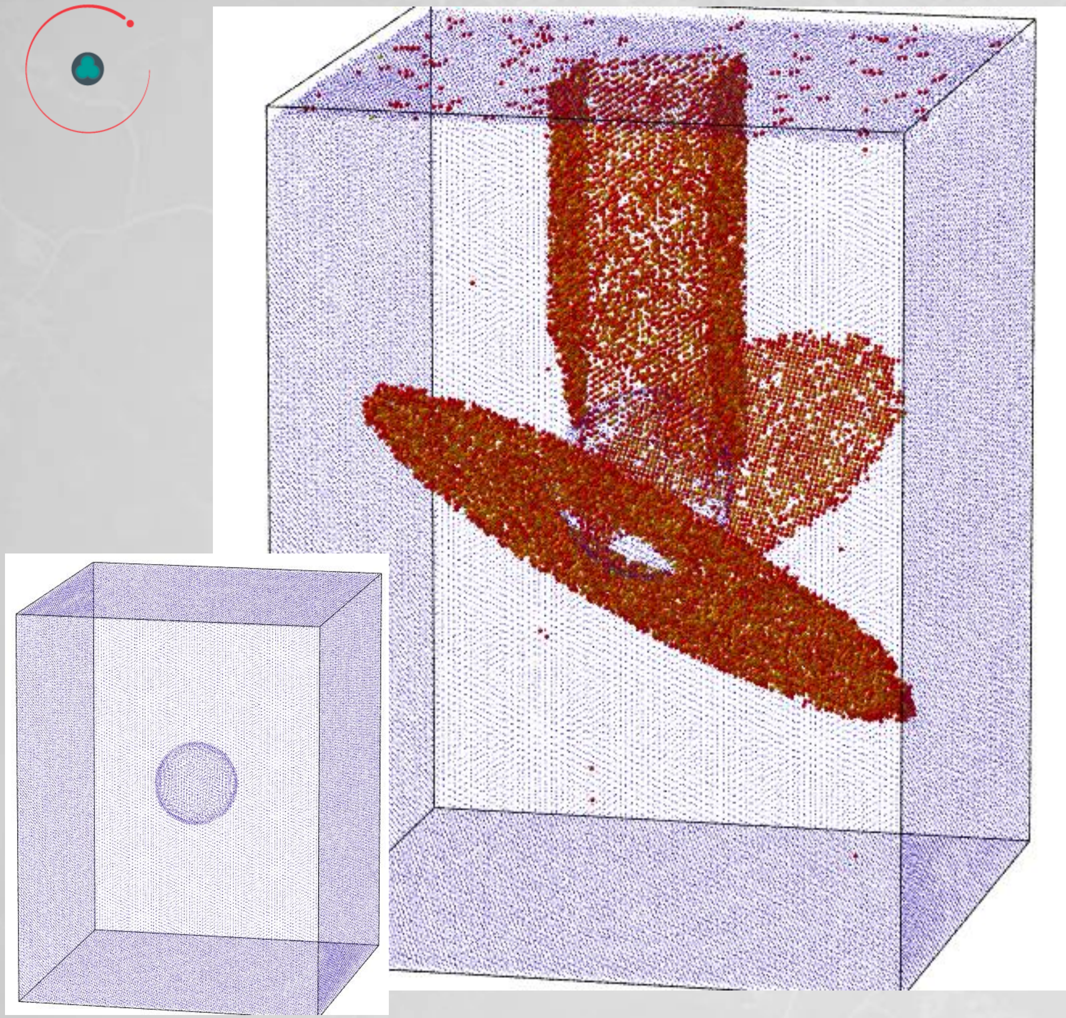
- The analysis of the protrusion height increase shows an asymptotic character. Once it starts growing, the self-reinforcing effect of the field enhancement around the tip of the protrusion causes the increase of its height in the "catastrophic" manner



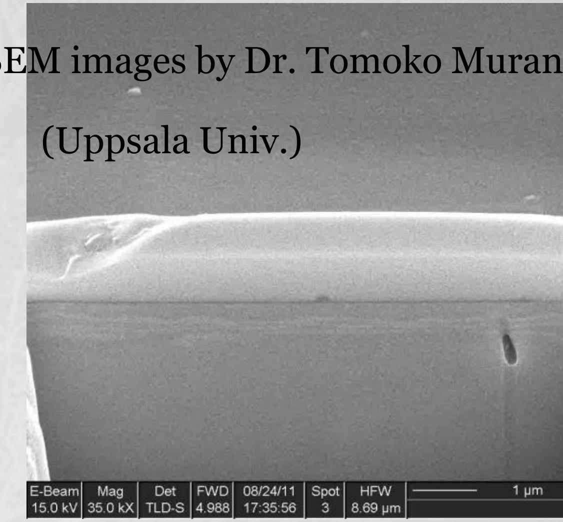

Experiment by Tomoko Muranaka, CERN

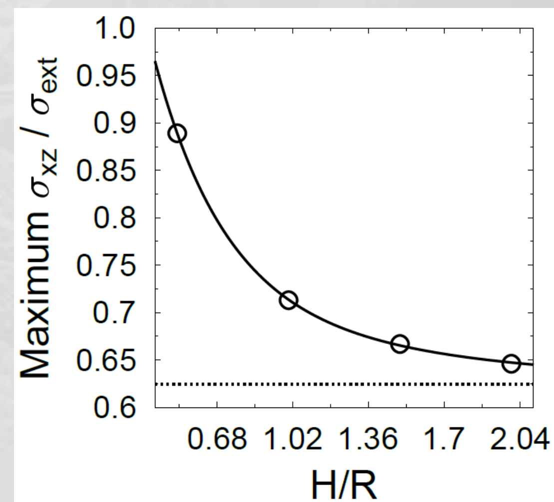
# Deeper under the surface



SEM images by Dr. Tomoko Muranaka

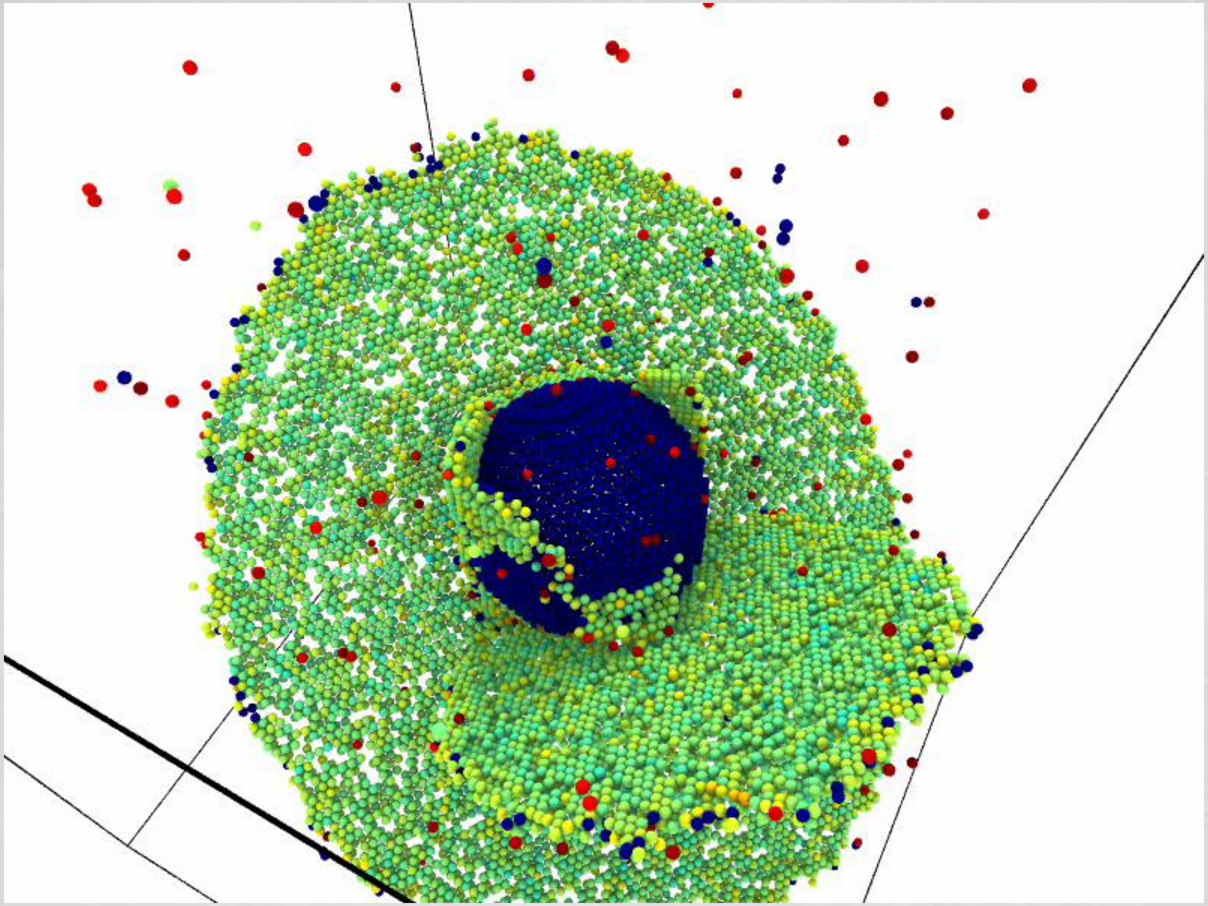
(Uppsala Univ.)




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

# Closer look at the void



- Size of the void is 4 nm, tensile stress is exaggerated, corresponding to 15 GV/m
- However, we did not expect a prismatic loop to be punched from a void

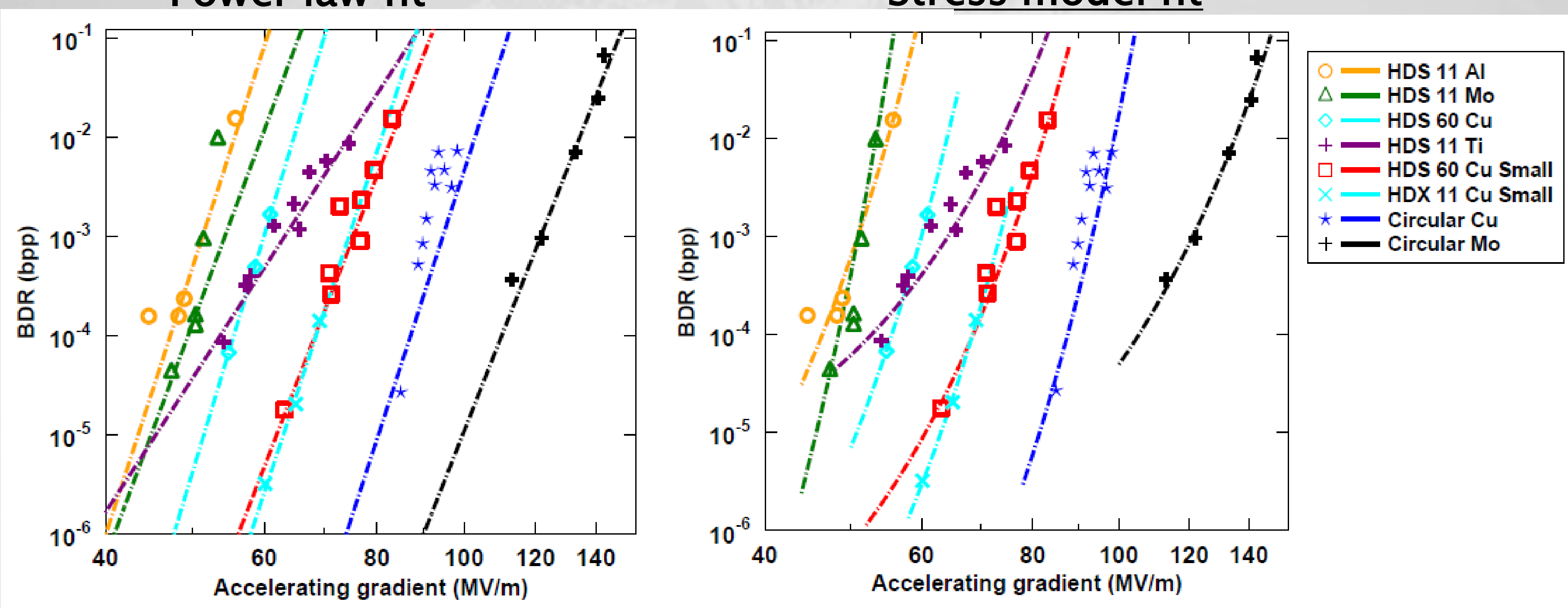
# Dislocation-based model for electric field dependence

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

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

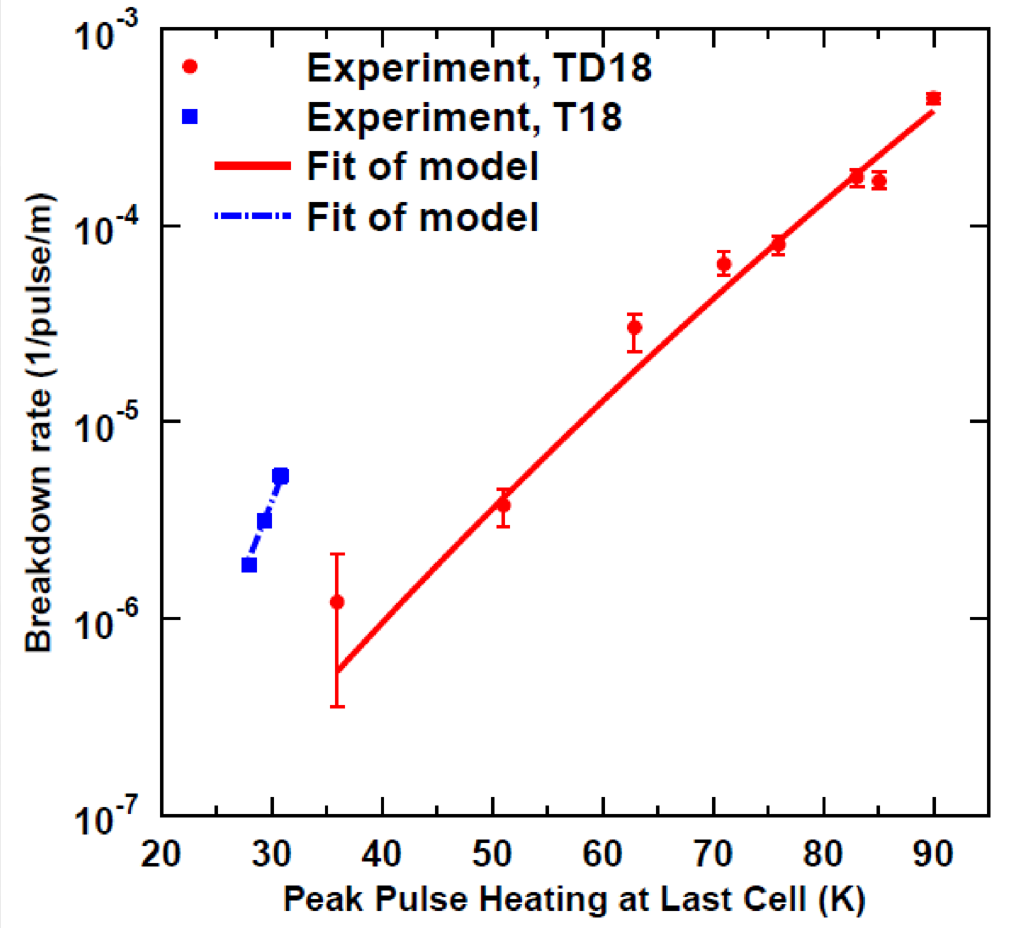
- Now to test the relevance of this, we fit the experimental data
- The result is:

**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

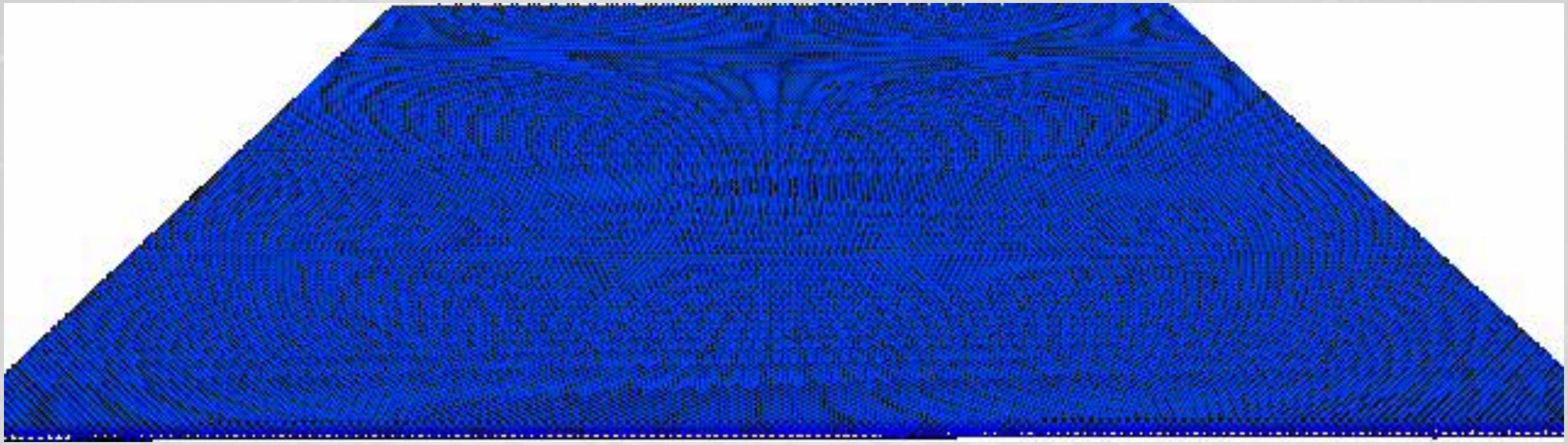
K. Nordlund and F. Djurabekova, Defect model for the dependence of breakdown rate on external electric fields, Phys. Rev. ST-AB 15, 071002 (2012).

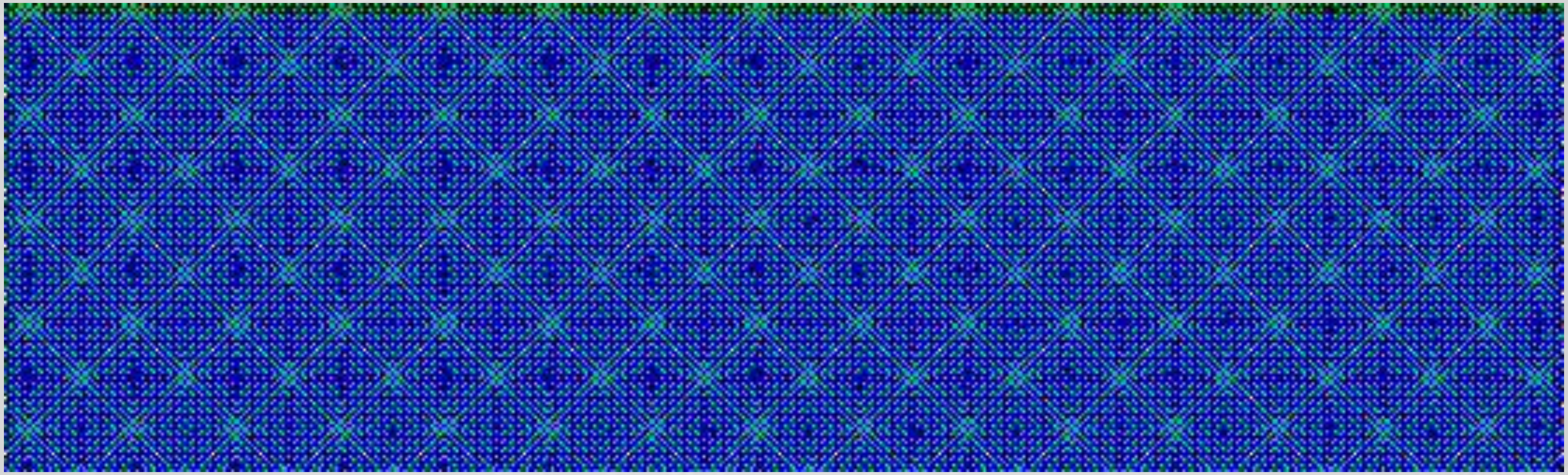
$$R_{BD} = a' c_0 \exp\left( \frac{-E^f + \varepsilon_0 E^2 \Delta V}{k_B (T_0 + \Delta T)} \right)$$

# Plasma impacts on Cu surface

- As plasma ion parameters we use the results obtained in 1D plasma claculations.
  - The merging of these simulations with 2D plasma development code is still in progress.
- To assess the effect of temperature and cooling we simulated three types of surfaces:
- Molten at melting point $T_m$
- Molten, just below $T_m$ (undercooled liquid)
- Still crystal,  just below $T_m$ (overheated crystal)
- Flux=4.9 x $10^{24}$ ions/cm$^2$/s
- Energy E=6 keV

# Plasma impacts: Arc-MD simulations

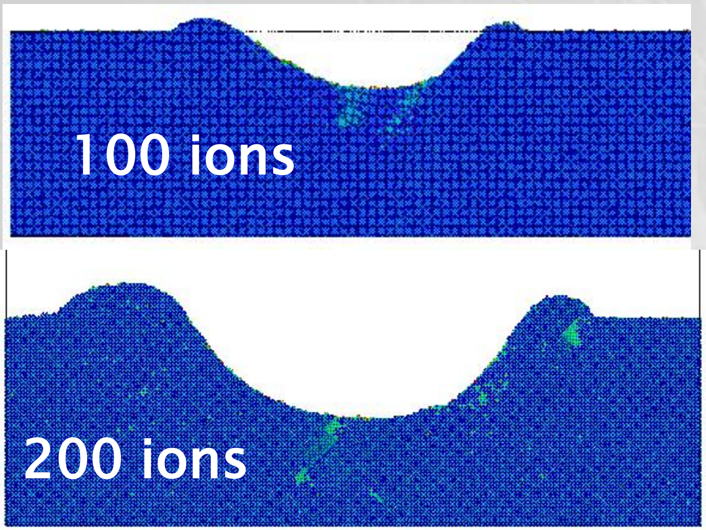




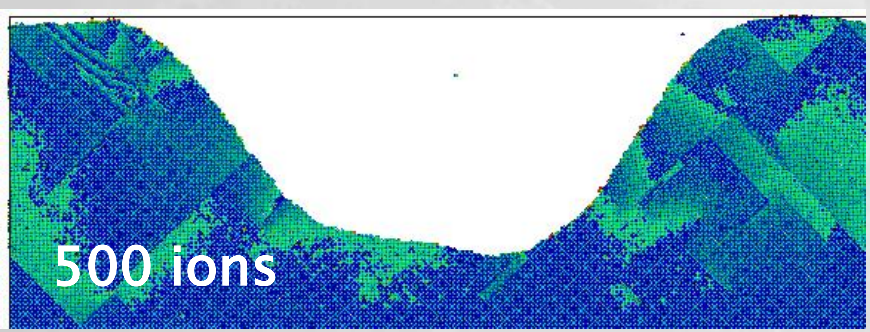
- The impact of 200 ions with the flux of $10^{24}$ ions $cm^{-2}s^{-1}$
- Energy of ions 6 keV at RT

# Changing fluxes

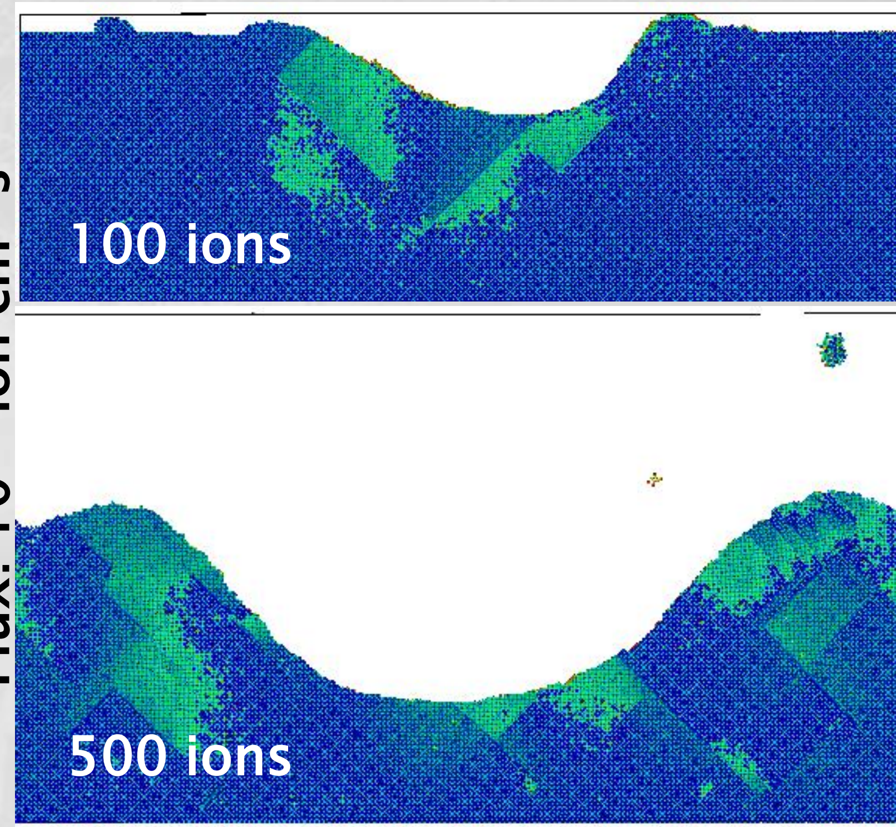
Flux: $10^{24}$ ion cm$^{-2}$s$^{-1}$




Flux: $10^{26}$ ion cm$^{-2}$s$^{-1}$

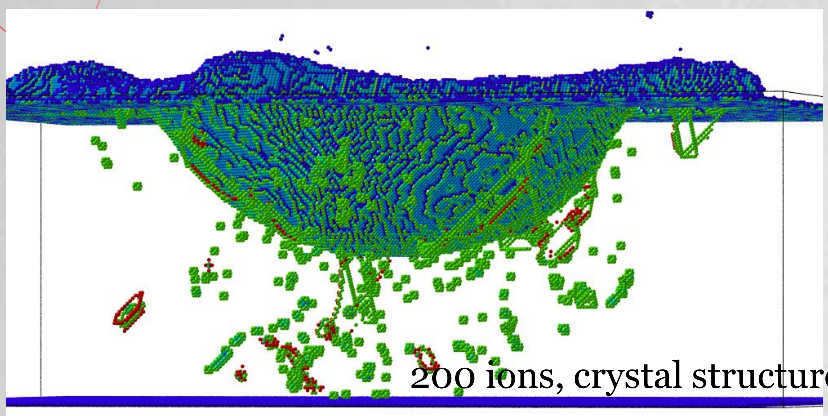



Flux: $10^{25}$ ion cm$^{-2}$s$^{-1}$

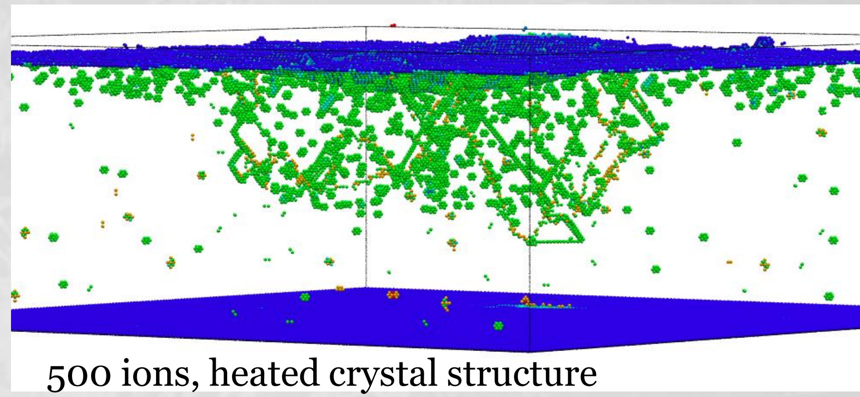



- Plastic deformations under the craters formed by plasma ions with different fluxes

# More detailed analysis under the breakdown spots

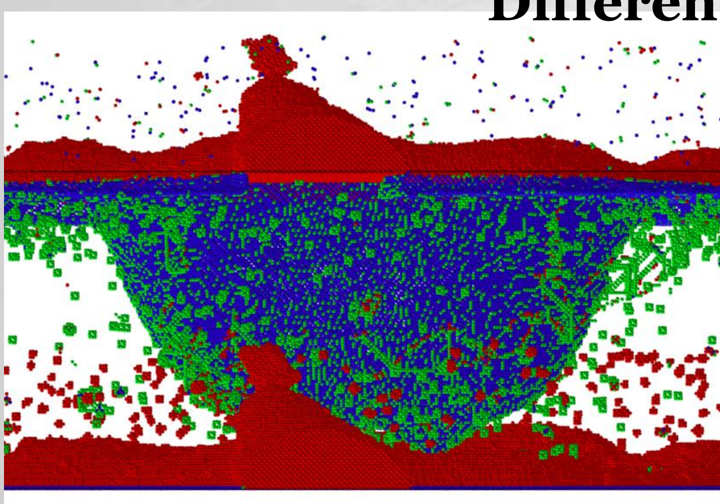


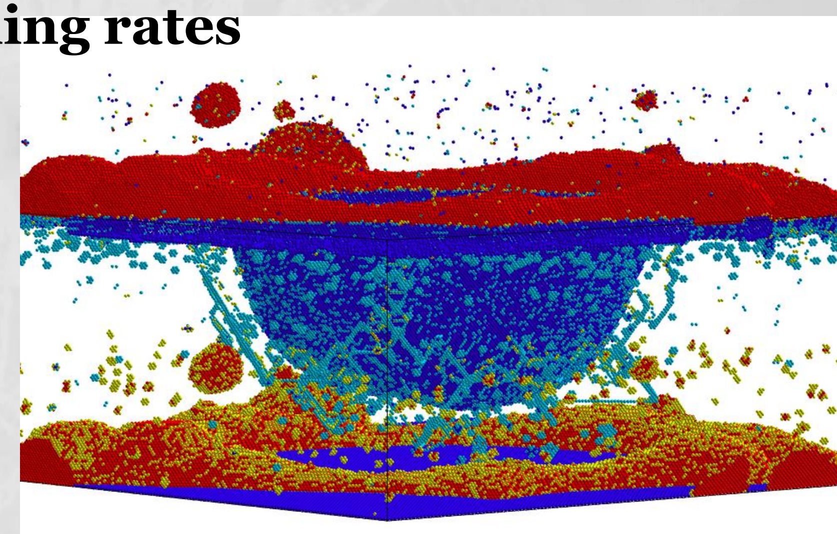
200 ions, crystal structure



500 ions, heated crystal structure

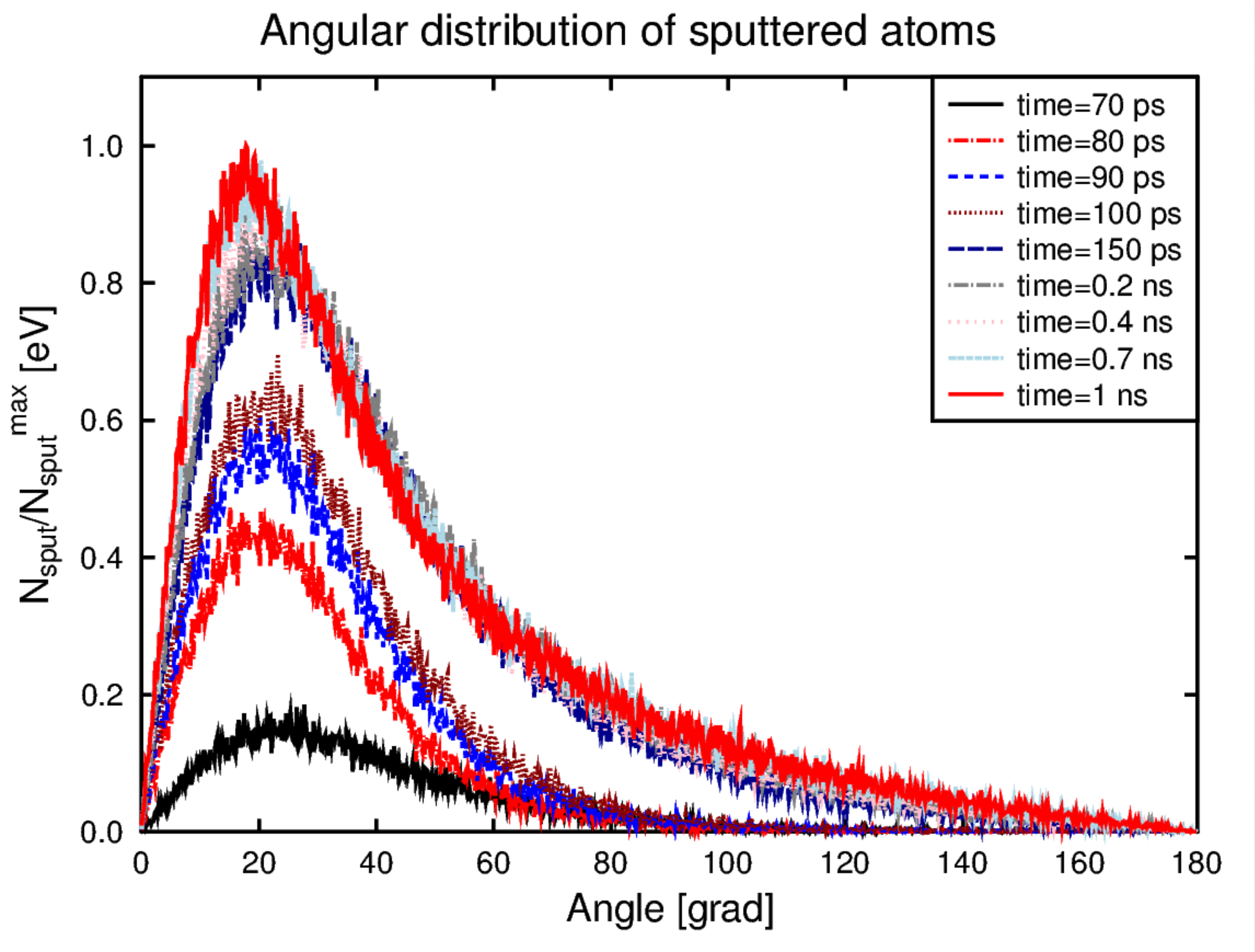
**Different cooling rates**





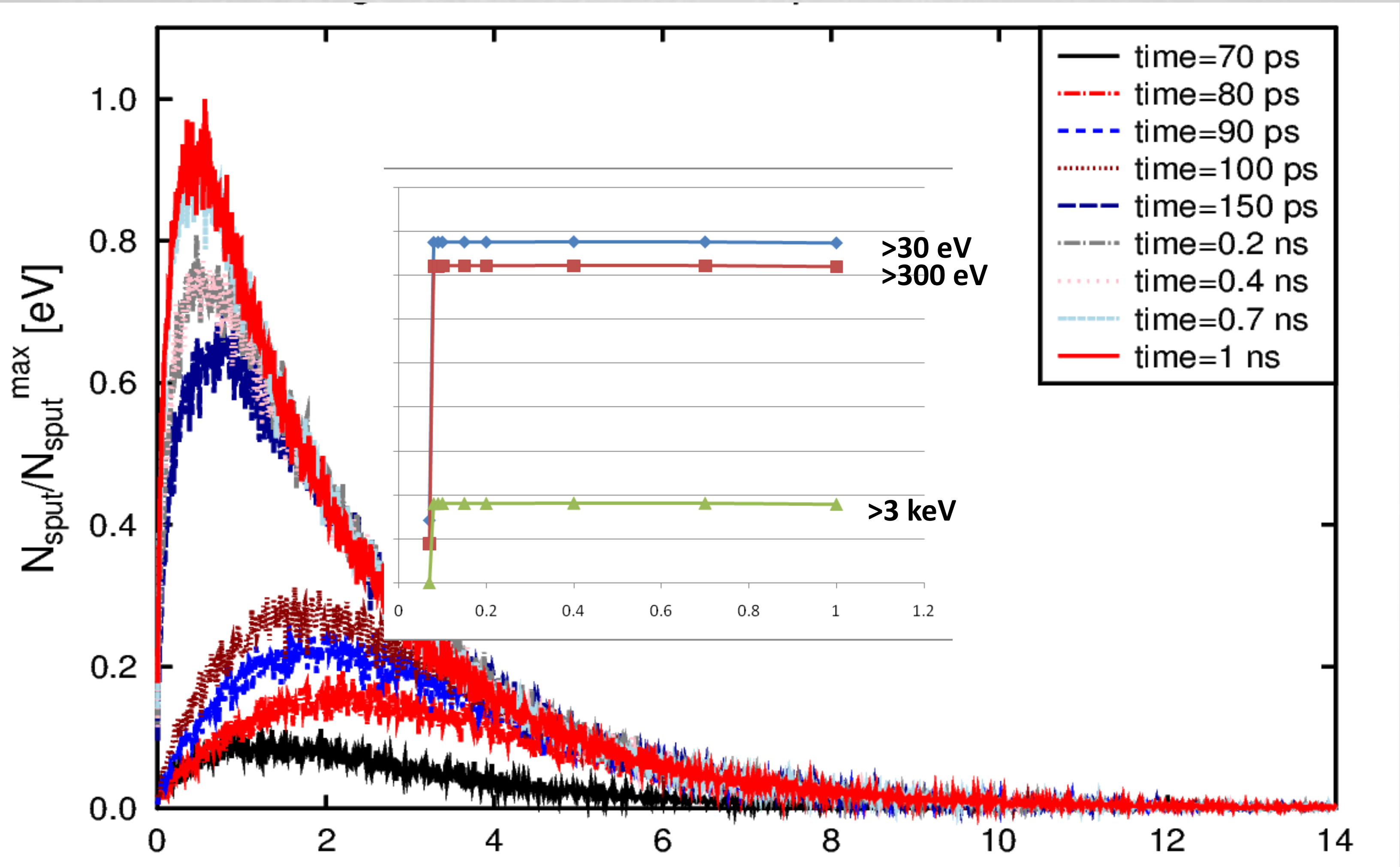
- We analysed a number of breakdown spots, there are many vacancies and small vacancy clusters as well as the dislocations under the impact spot

# Analysis of the sputtered atoms




- Angular distributions of sputtered atoms, some atoms turn back to the surface (~180°)

# Energy distribution




- Mostly the atoms are sputtered with the thermal energies less than 2 eV,

# 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 participate in the formation of extended defects for future emitting spots.

# Thank you for attention and valuable feedback!