HELSINGIN YLIOPISTO
HELSINGFORS UNIVERSITET
UNIVERSITY OF HELSINKI

HIP

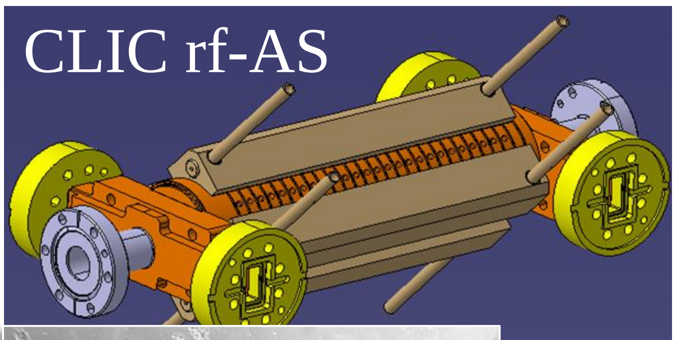
Multiphysics simulations of onset of vacuum electrical breakdowns

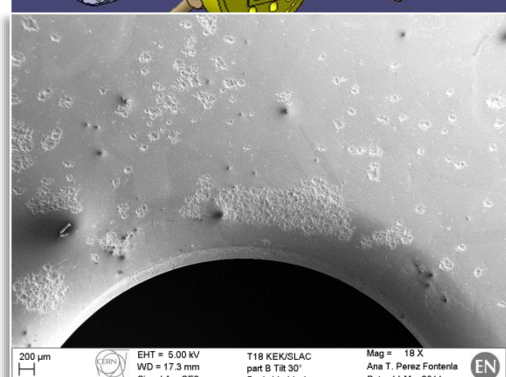
Flyura Djurabekova

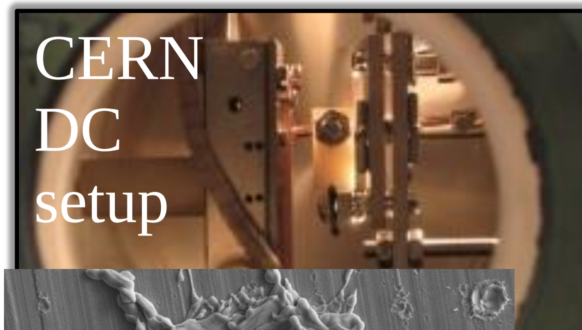
Helsinki Institute of Physics and Department of Physics
University of Helsinki
Finland

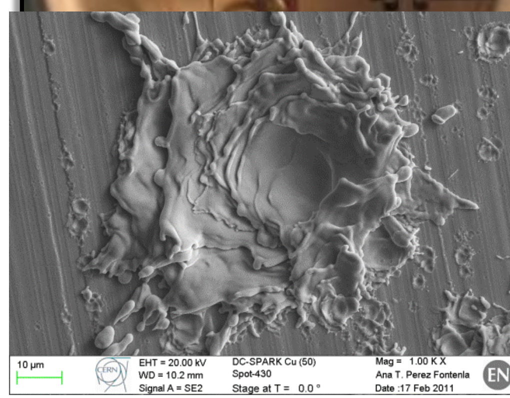
Breakdowns in ultra high vacuum

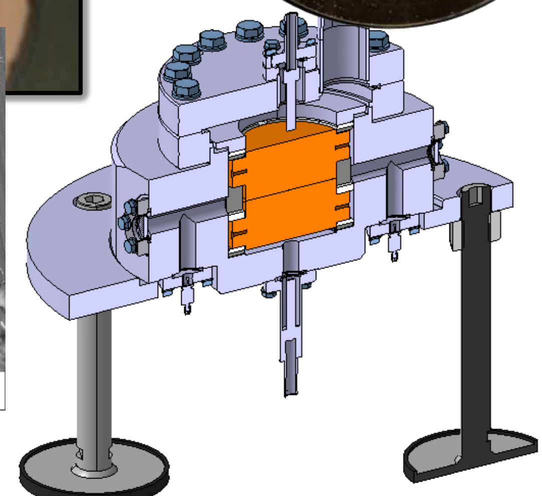
- We are developing the model, which will be able to describe the processes involved in the processes of electrical breakdowns in rf and dc-fields.







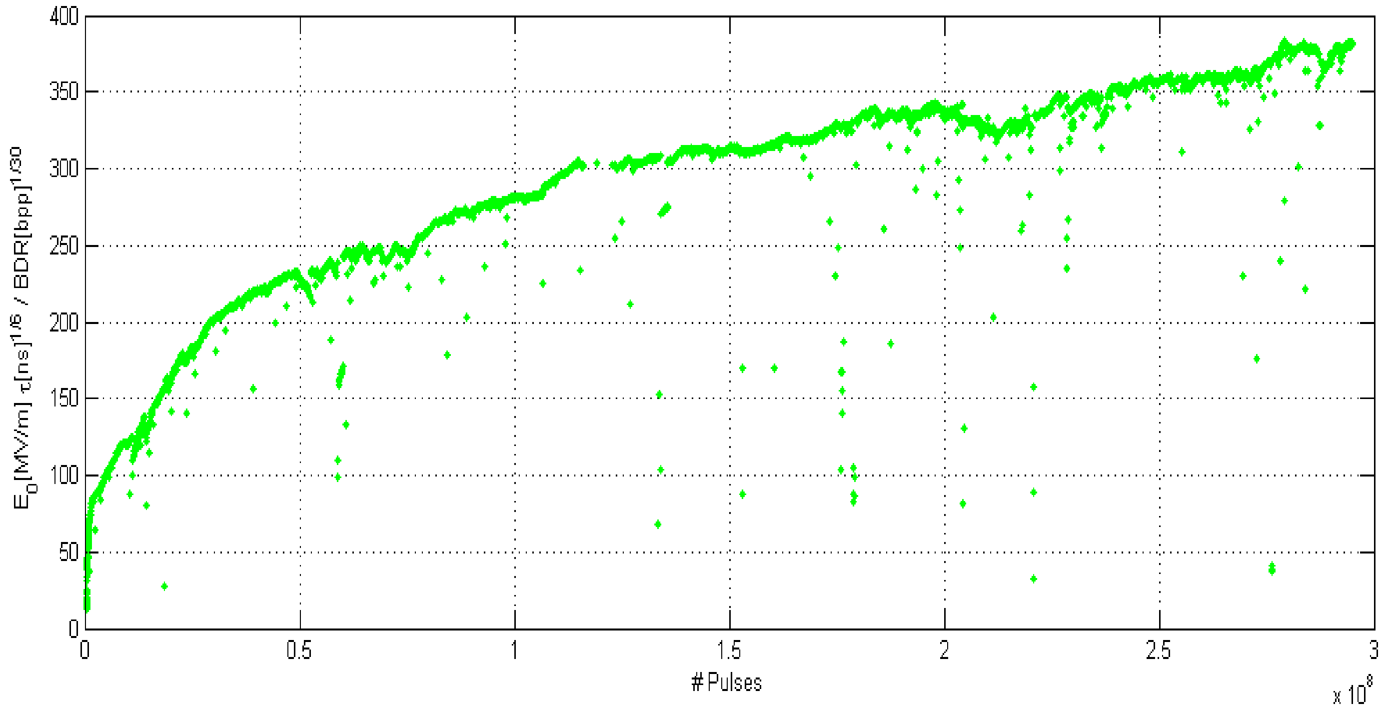




Conditioning history of AS at CERN

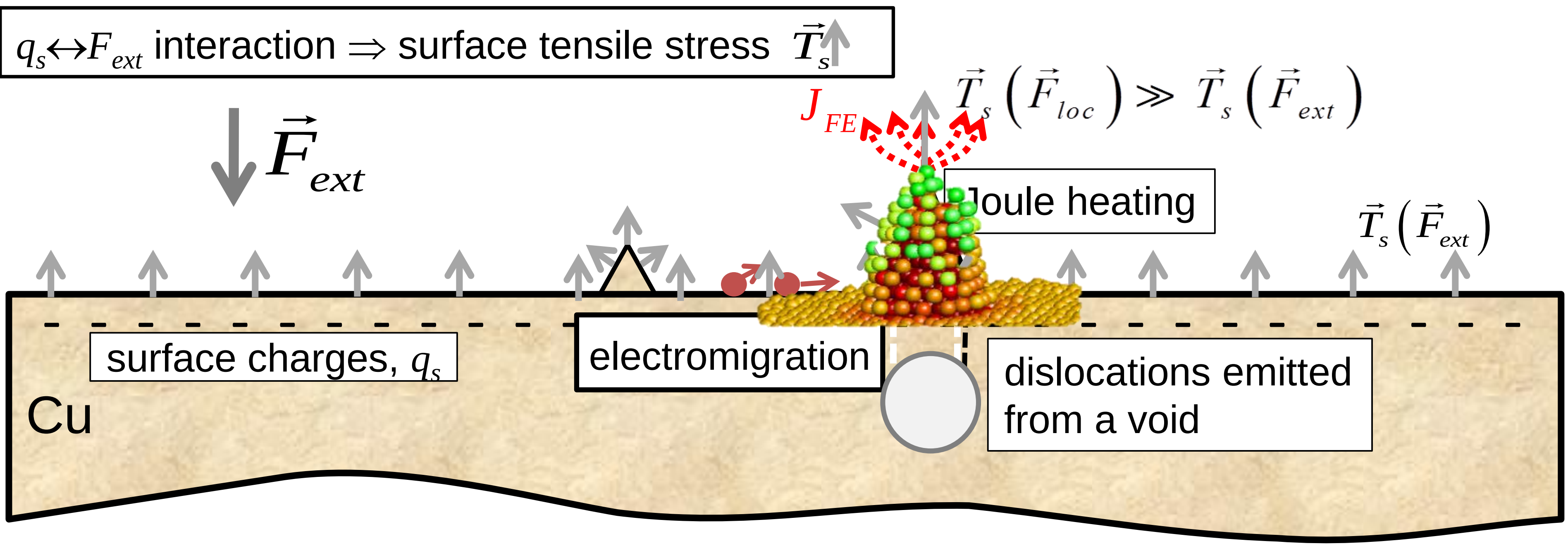
11168 BDs

- CERN TD26R05CC conditioning history plot



The conditioning behaviour of a CLIC prototype accelerating structure. The time corresponds to over four months of operation at 50 Hz. The vertical scale is the accelerating gradient normalized for pulse length and breakdown rate.

Mechanisms *on* and *under* the surface in the presence of electric fields

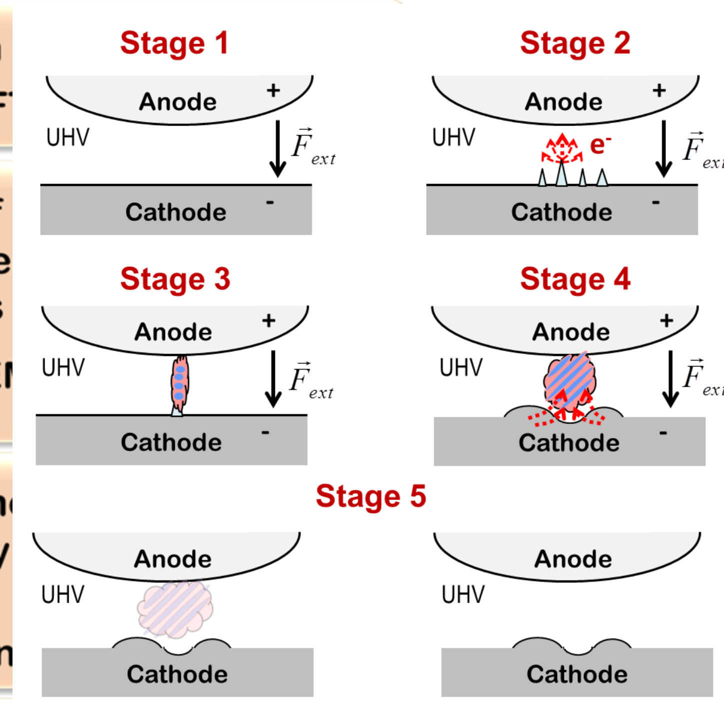


ultiphysics model

Stage 1 Charge on
Method: SIESTA (DF

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

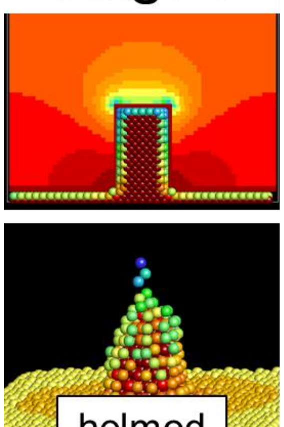
Stage 2b Long tim
surface morphology
surface charge
Method: kimocs (Kin



Stage 3 Field assisted evaporation of
ns & Jo ectromig
FE currents

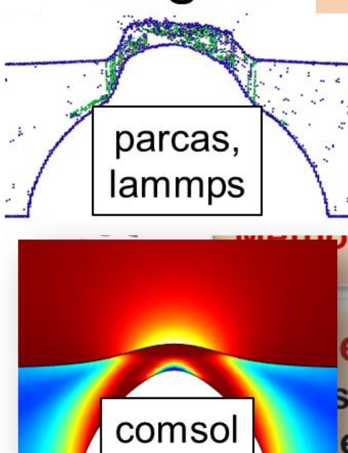
e ion bombardment from
eating b ents
Method: Arc MD

Stage 1



helmod

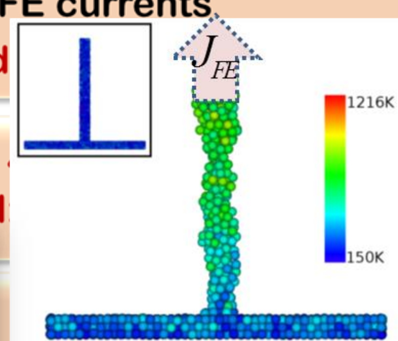
Stage 2



parcas, lammps

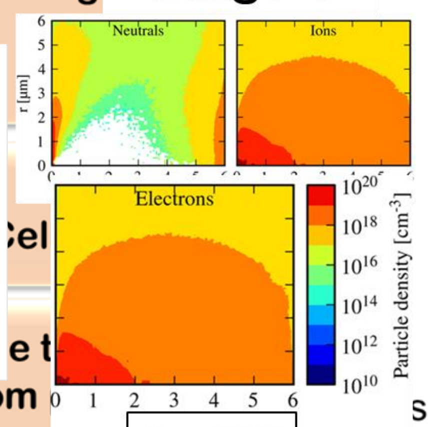
comsol

Stage 3



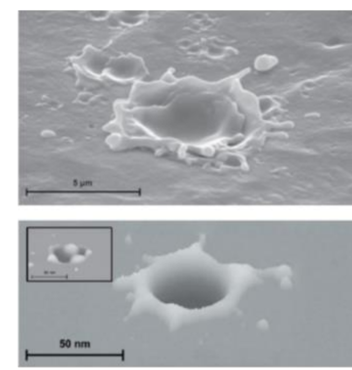
helmod

Stage 4



Arc-PIC

Stage 5



Arc-MD

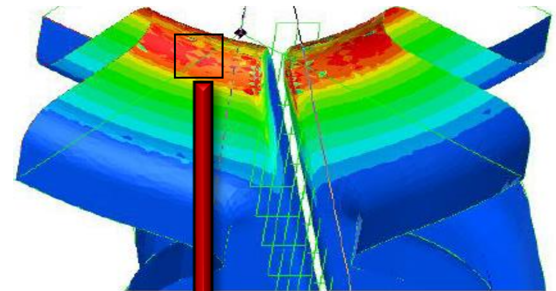
External electric field in MD simulations

- Gauss law by 'pllbox' technique

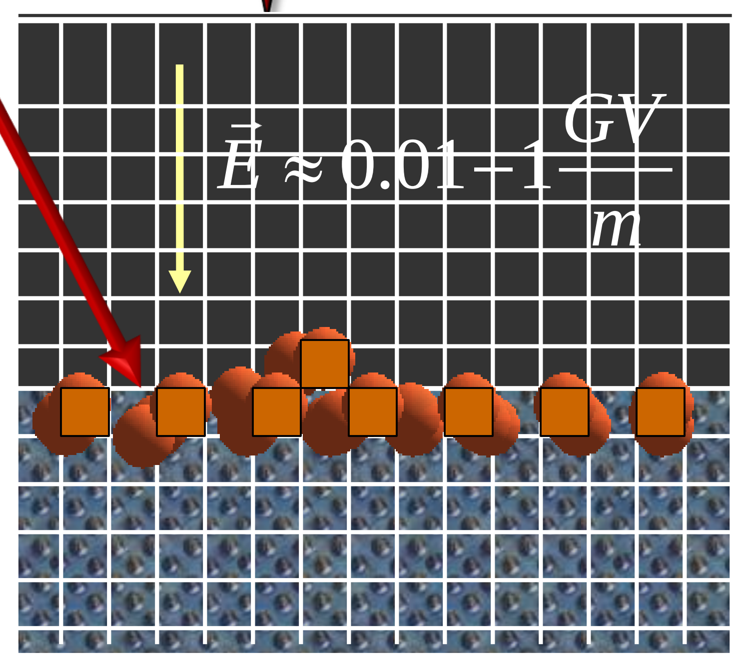
$$\sigma = \frac{Q_{surface}}{A_{surface}} = \varepsilon_0 E$$

Due to the external electric field the surface attains charge

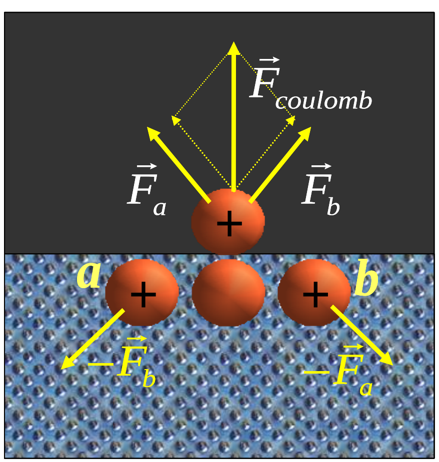
Macroscopic field to…



…the atomic level:



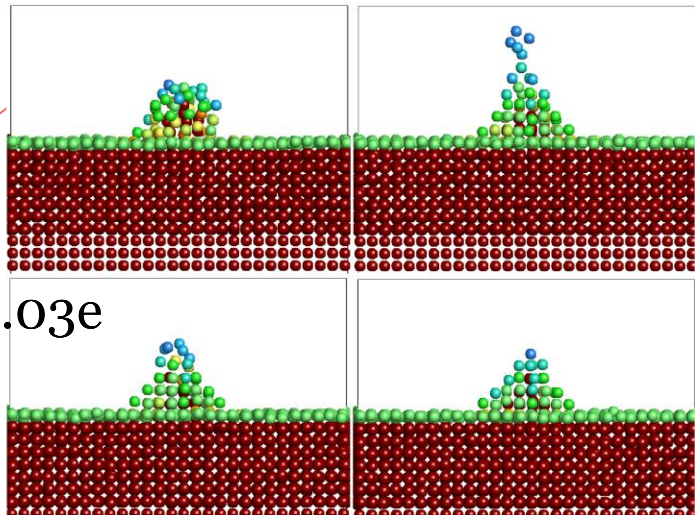
Two electric forces modify the motion of charged atoms:



$$\vec{F}_L = \vec{E}q$$

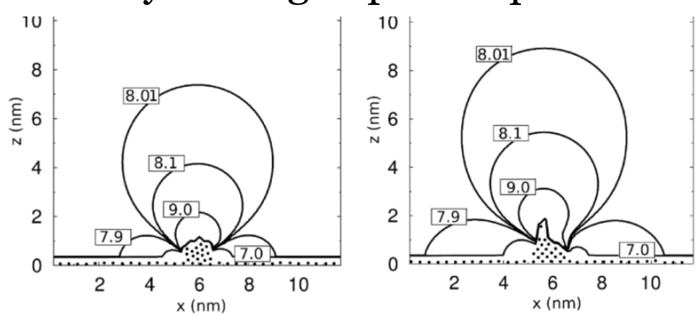
$$\vec{F}_C = \frac{1}{4\pi\varepsilon_0}\sum_i \frac{q_a q_i}{r_{0i}^2}\hat{r}_{0i}$$

Charges on surface atoms in MD



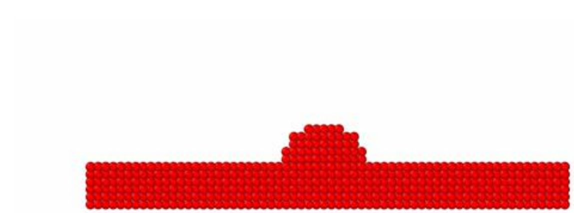
$q_{at} \leq 0.03e$

Distribution of the electric field is dynamically calculated by solving Laplace equation



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

- Charges on surface atoms are calculated by using our ***helmod*** code – hybrid ED-MD code, based on classical MD (molecular dynamics) code.
- The dynamics of atom charges follows the shape of electric field distortion on tips on the surface
- The atoms leave the tip as a result of evaporation enhanced by pulling effect from the external electric field.
  - No electromigration or interaction with electrons are taken into account so far



Helmod *vs* SIESTA

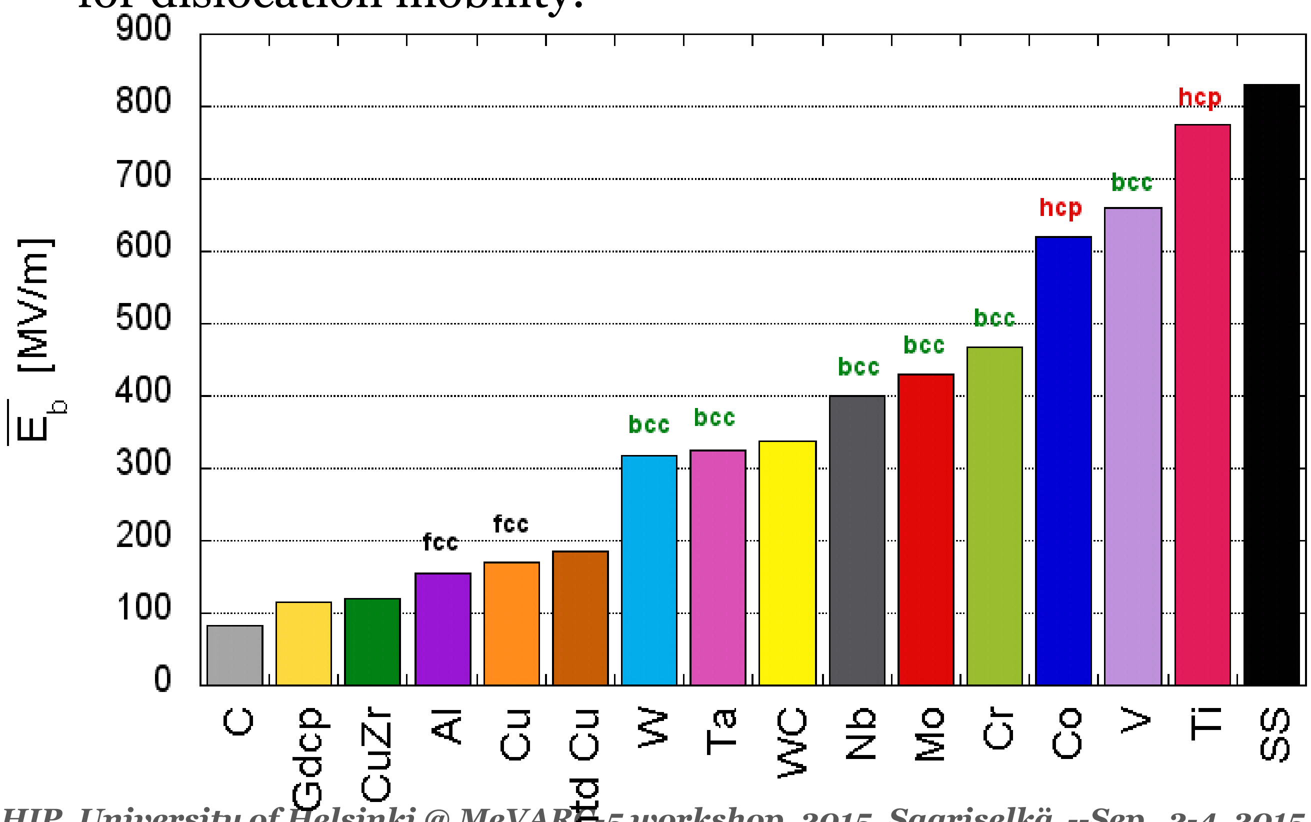
- Comparison of the results of both approaches gives reasonable agreement

Defect	Helmod	DFT, SIESTA
An adatom	0.043e	0.034e
Double adatom	0.035e	0.025e
A vacancy	0.009e	0.014e
Double vacancy	0.01e	0.013
4 vacancy	0.01e	0.01e

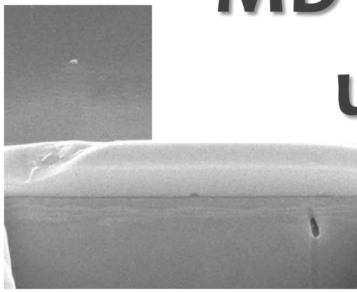
What are the field emitters? Motivation to look in under the surface

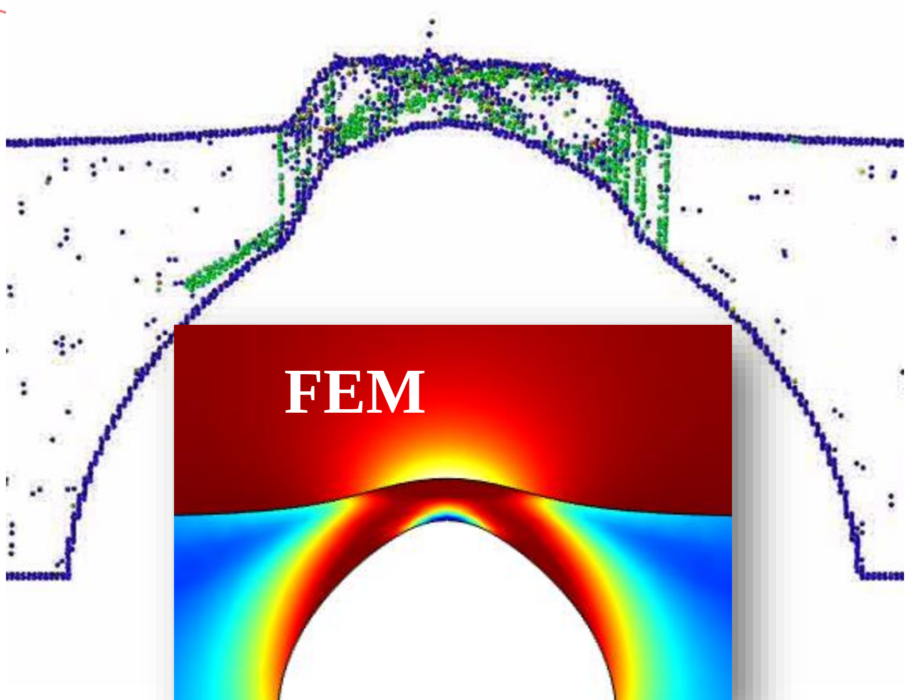
- The dislocation motion is strongly bound to the atomic structure of metals. In FCC (face-centered cubic) the dislocation are the most mobile and HCP (hexagonal close-packed) are the hardest for dislocation mobility.

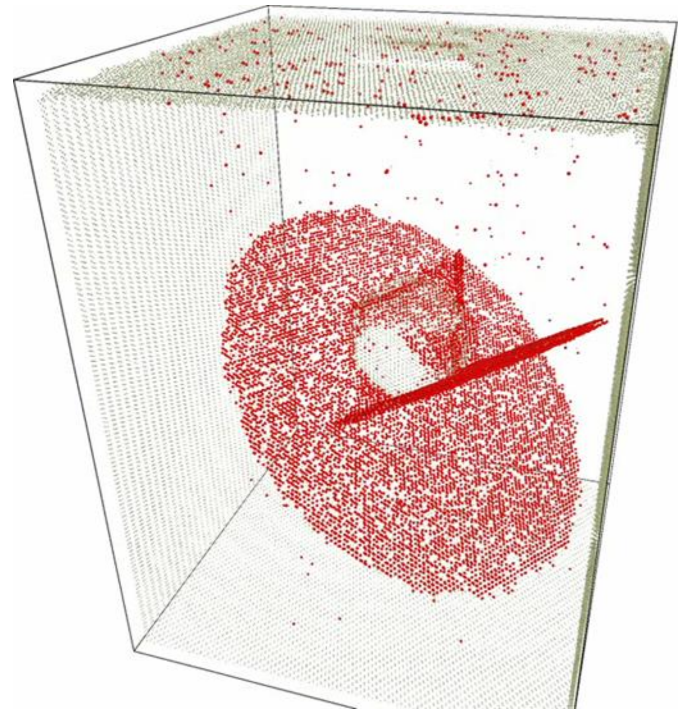
A. Descoeudres, F. Djurabekova, and K. Nordlund, DC Breakdown experiments with cobalt electrodes, CLIC – Note – 875 , 1 (2010).



MD simulation of plastic activity under a high electric field





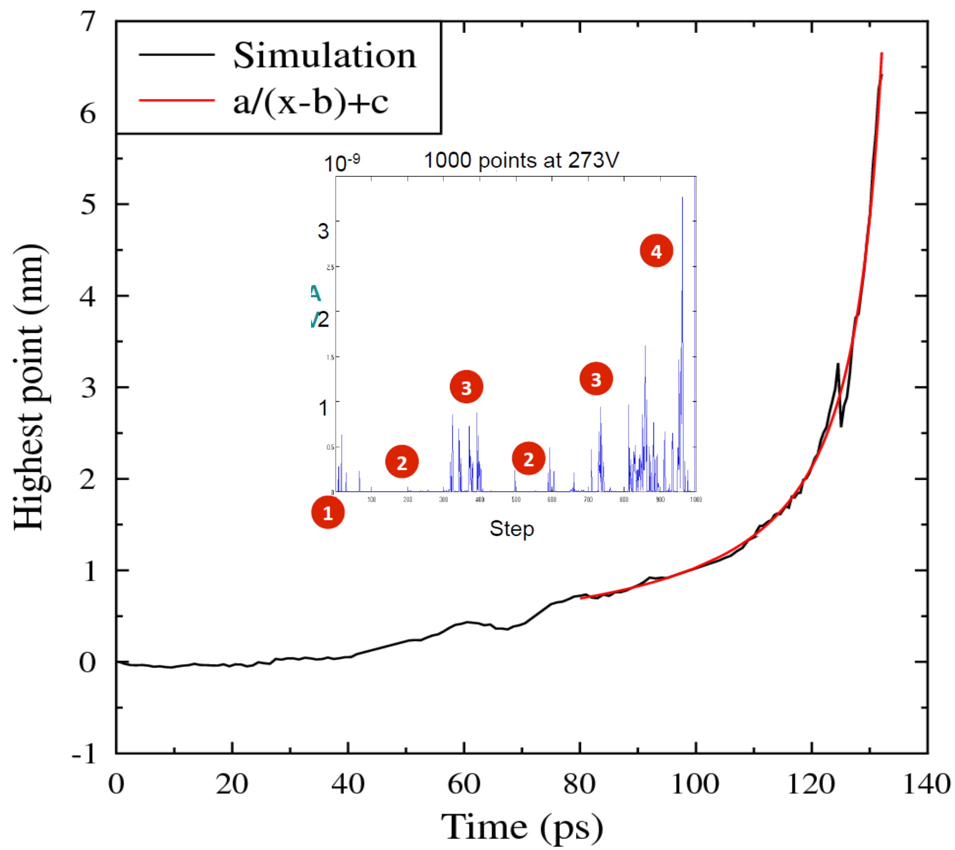


- Behavior of a void under tensile stress due to an electric field (Simulations are done with the ***helmod*** code, where the electric field effect is accounted explicitly)

MD in [A. S. Pohjonen, S. Parviainen, T. Muranaka, and F. Djurabekova, JAP 114, 033519 (2013)]
FEM in V. Zadin, A.Pohjonen, A. Aabloo, K. Nordlund, and F. Djurabekova, Phys. Rev. ST-AB (2014),

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

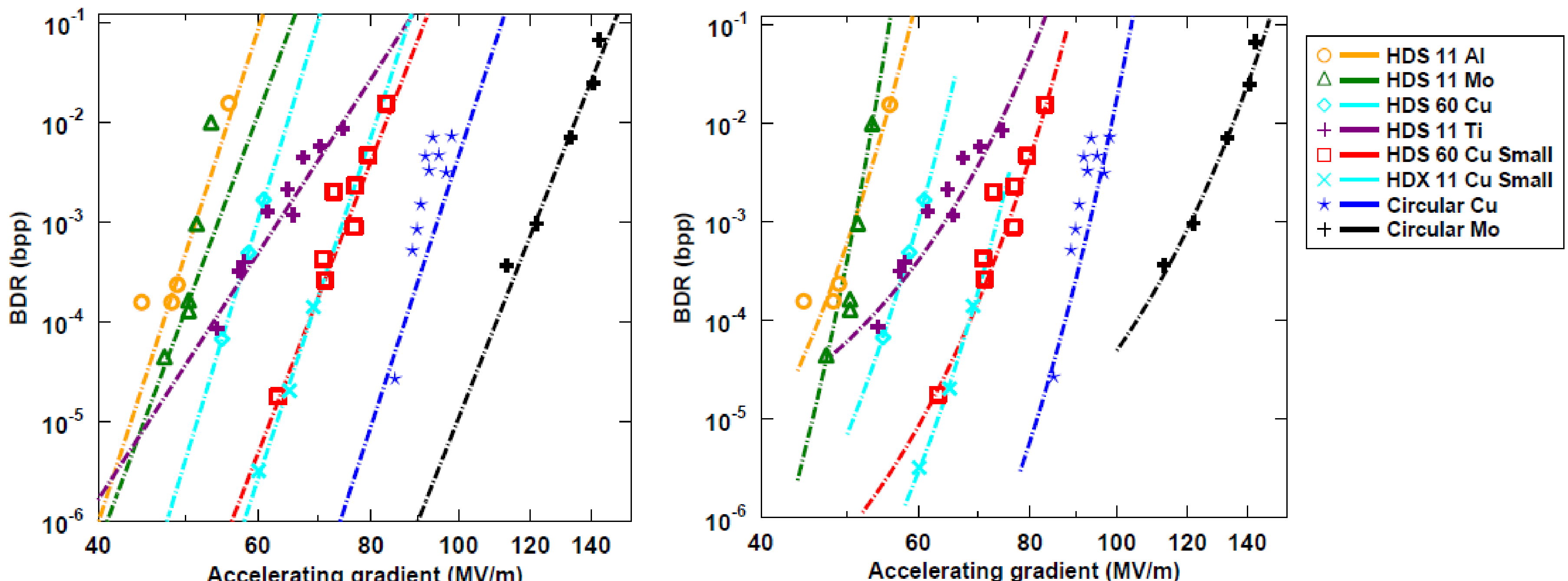
Dislocation-based model for electric field dependence

- 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**

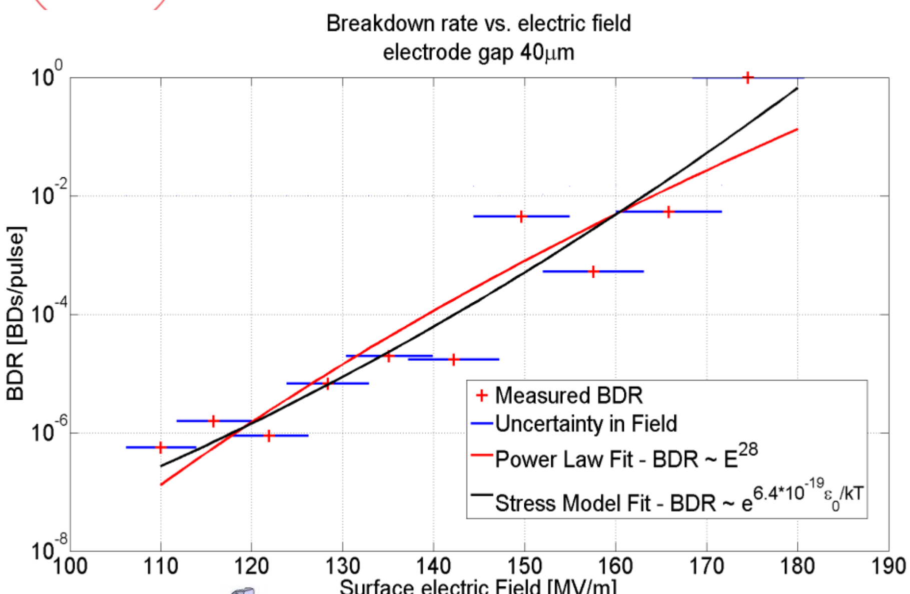


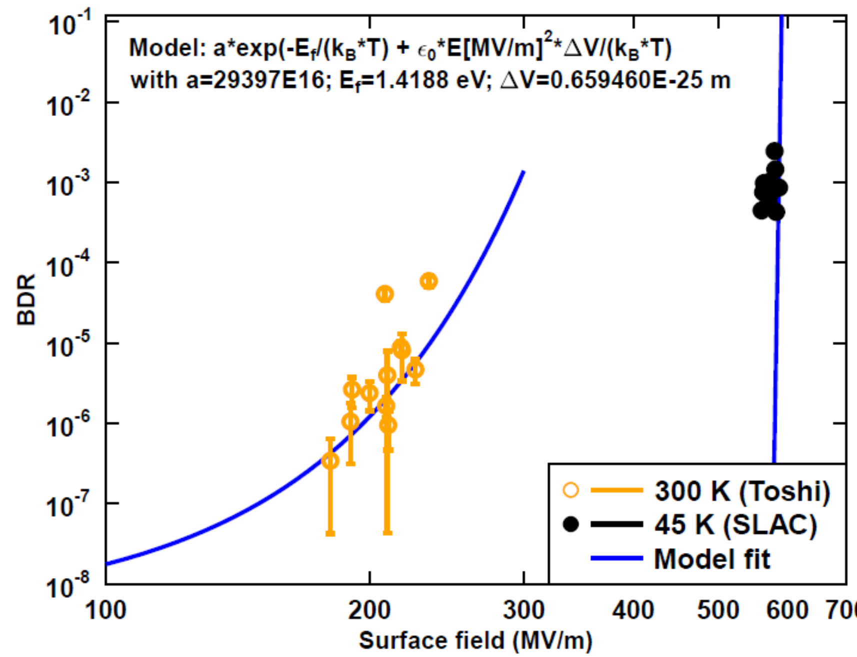
[W. Wuensch, public presentation at the CTF3, available online at http://indico.cern.ch/conferenceDisplay.py?confId=8831.] with the model.]

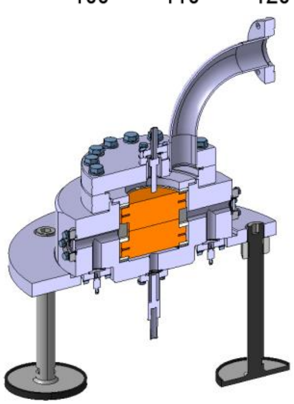
K. Nordlund and F. Djurabekova, Phys. Rev. ST-AB 15, 071002 (2012).

More data fit to the model

BDR in the pulsed dc (CERN)



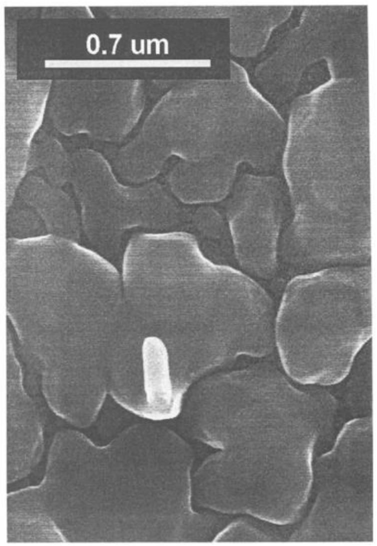




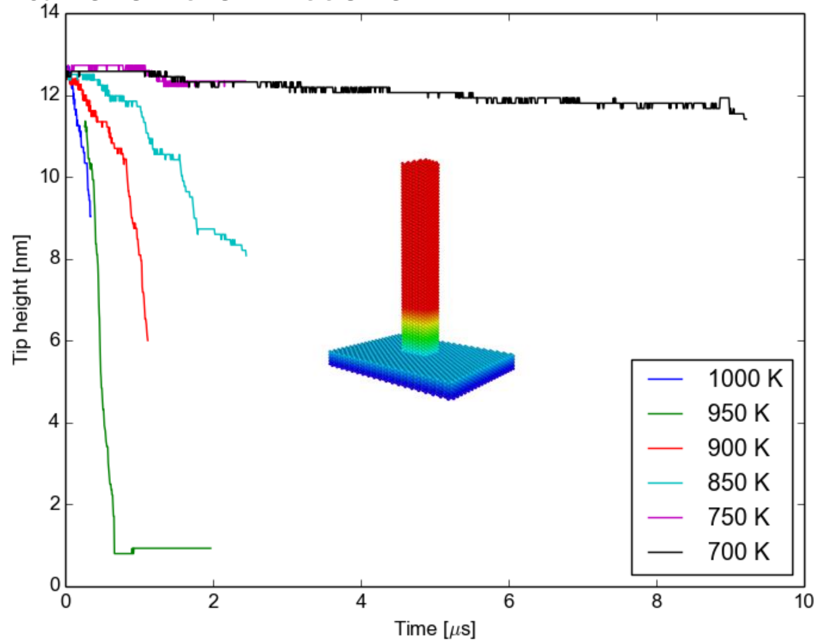
- Pulsed DC experiments also give a good agreement with the model.
- As a preliminary test, we found that the same fitting parameters can reproduce both data taken from KEK (300K) and SLAC (45K) experiments.

Stability of tips

- By using different methods (MD, see talk by M.Veske and KMC, see talk by V.Jansson) we are analyzing the stability of the nanometric tips which can be the building up transient emitters



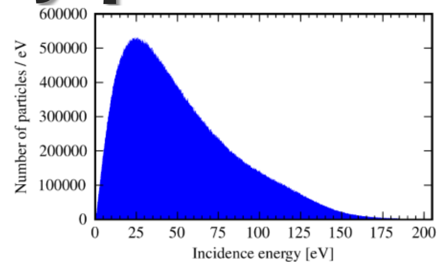
Copper tips with R <120 nm and H >300 nm have been found to be stable for months at RT

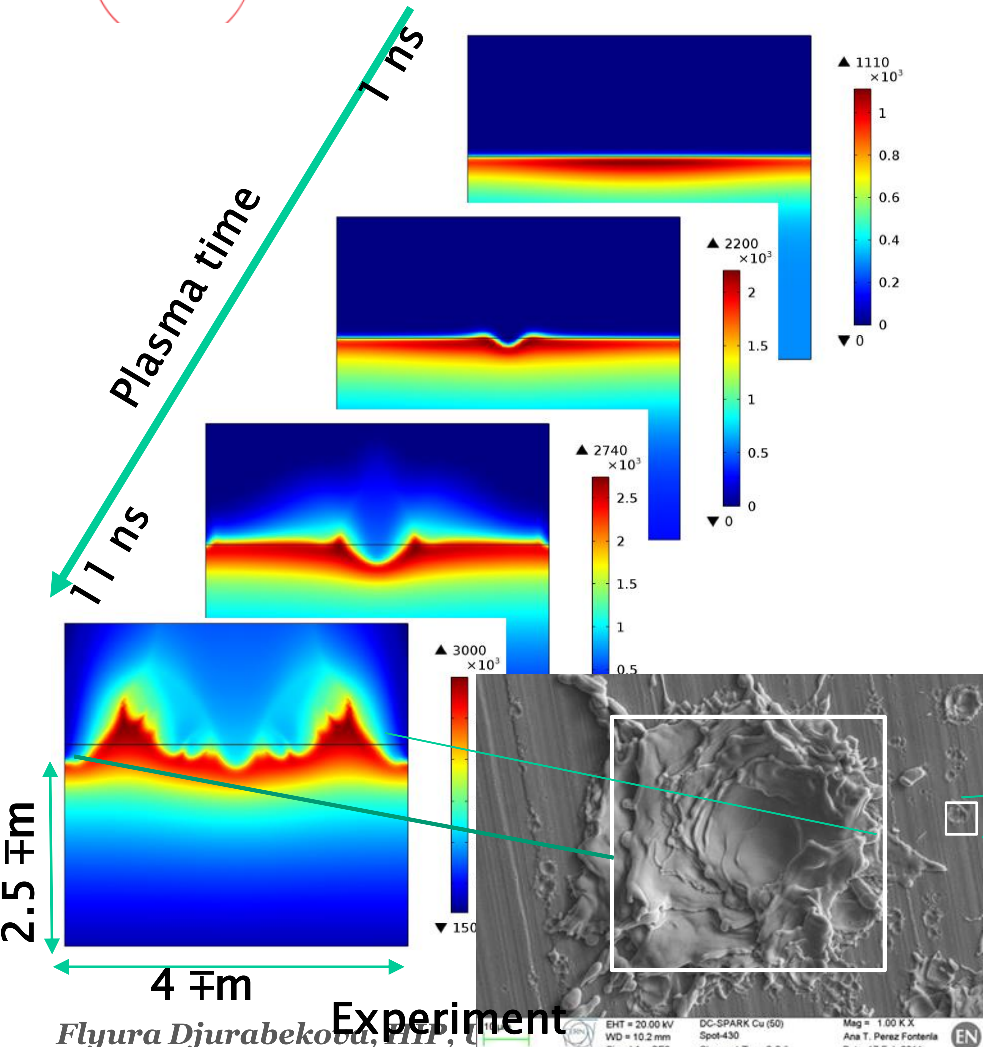


- The height of the tip is as a function of time. At 300 K, the height was still unchanged after 10 ms.

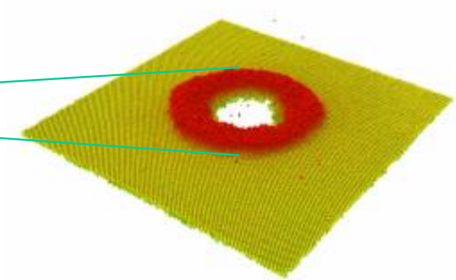
Surface damage by plasma ions

Plasma ions (from actual PIC calculations):
E_{ion} = 55 eV
flux = $5x10^{24}$ ion $cm^{-2}s^{-1}$





- By combining two methods, MD and FEM, we can clearly distinguish between the regimes of crater formation and splashes (liquid phase instabilities) after the breakdown event (left).
- Small size craters can be formed by the undeveloped plasma (sputtering yield (atom/ion) is less than 1) (bottom left)



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
- Long term surface evolution is added into the model.
- Surface damage formation is receiving a new perspectives

Thanks to:

- Group in Helsinki
  - Postoctoral researchers:
    - Dr. Stefan Parviainen
    - Dr. Ville Jansson
    - Dr. Vahur Zadin (Tartu Univ.)
  - Former group members:
    - Dr. Aarne Pohjonen
    - Dr. Helga Timko
    - Dr. Lotta Mether
  - PhD students
    - Avaz Ruzibaev
    - Simon Vigonski (Tartu Univ.)
    - Mihkel Veske (Tartu/Helsinki)
    - Ekaterina Baibuz
    - Mrunal Parekh

- Collaborators and colleagues
  - Helsinki:
    - Prof. Kai Nordlund
    - Dr. Antti Kuronen
    - Dr. Kenneth Österberg
  - **CERN**:
    - Dr. Walter Wuensch
    - Sergio Calatroni
    - Kyrre Ness Sjoebaek
  - Hebrew university of Jerusalem
    - Dr. Yinon Ashkenazy

You can find more information at
http://research.hip.fi/hwp/acctech/accelerator-technology/m-a-t/

Thanks to:

http://research.hip.fi/hwp/acctech/accelerator-technology/m-a-t/