

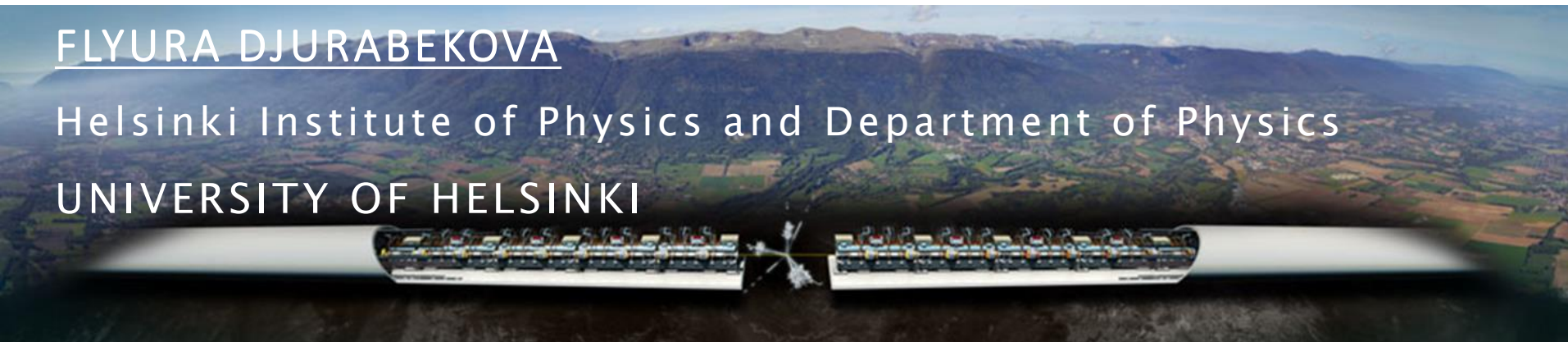


Atomistic approach in understanding of mechanisms leading to vacuum arcing

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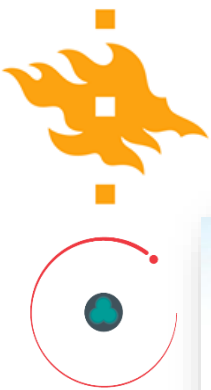
UNIVERSITY OF HELSINKI



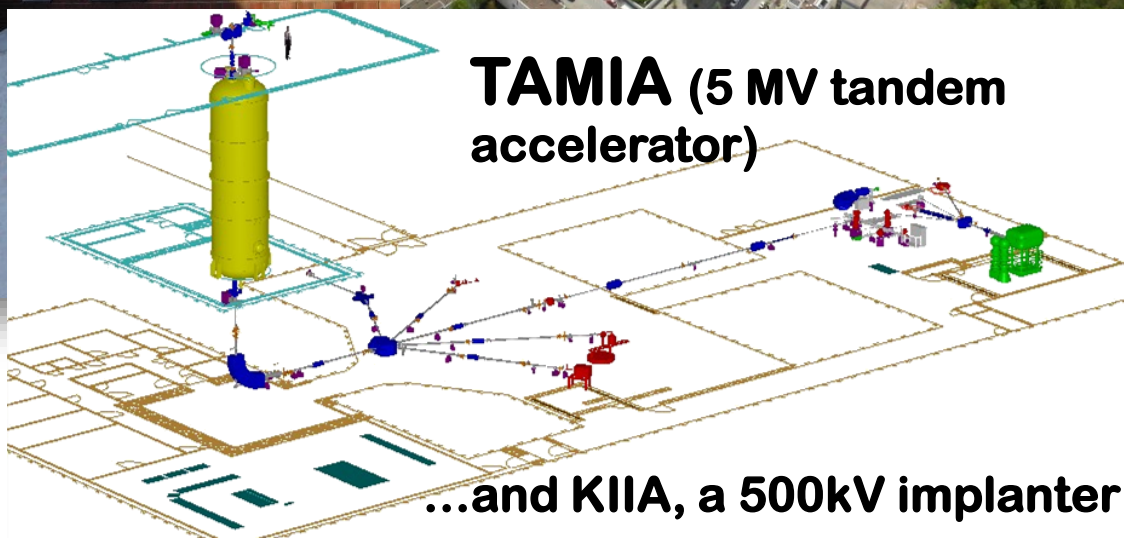
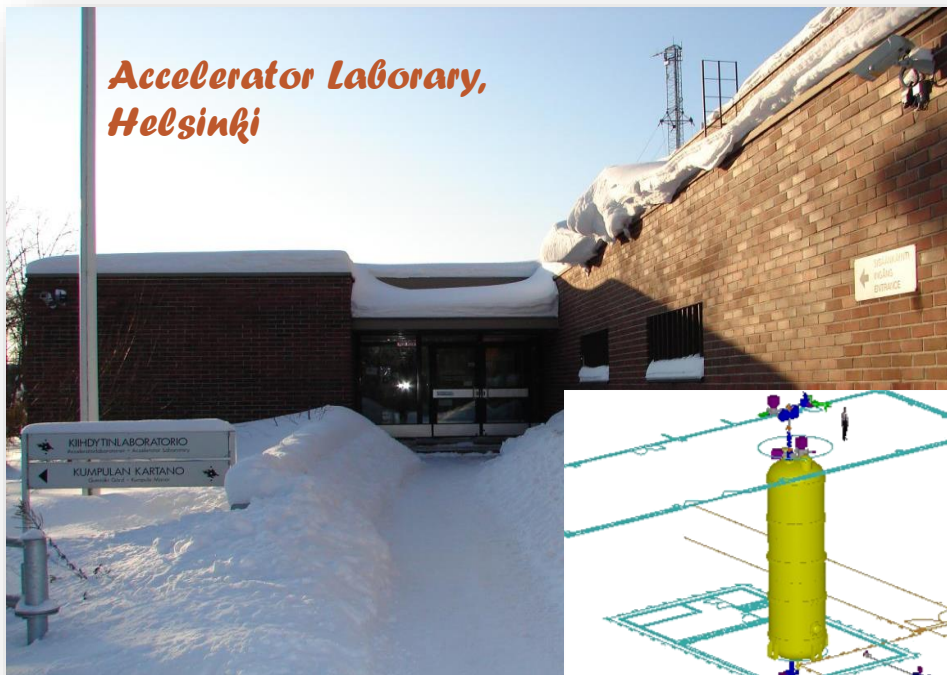


Where we are from:





Helsinki Accelerator Laboratory (HAL)

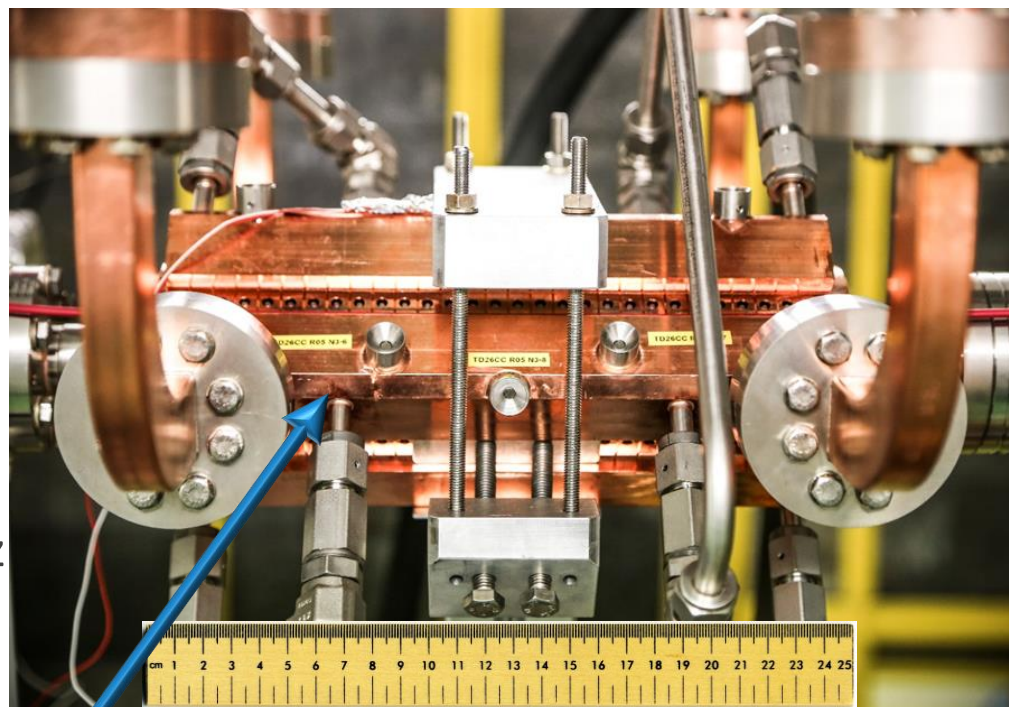


<https://www2.helsinki.fi/en/researchgroups/helsinki-accelerator-laboratory>

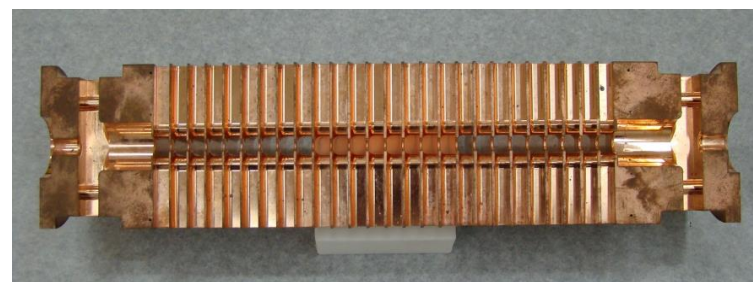
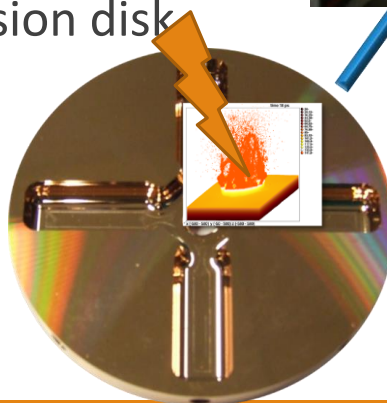


Accelerating structures – main component of CLIC

- 11.994 GHz, X-band
- 100 MV/m accelerating gradient
- Input power ≈ 50 MW
- Pulse length ≈ 200 ns
- Repetition rate 50-400 Hz



Micron-precision disk



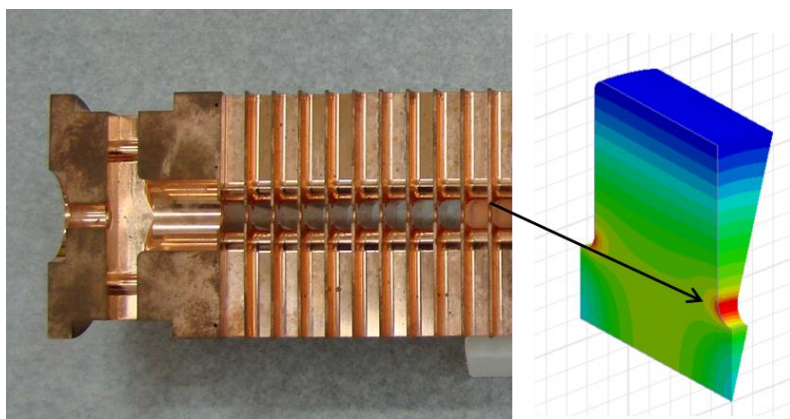


What is the main physical limitation?

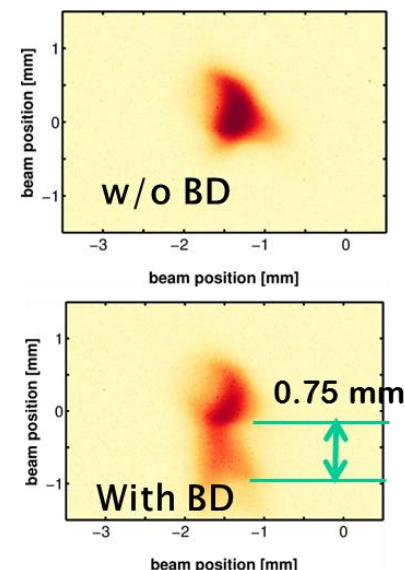
Vacuum breakdown

An accelerating gradient of 100 MV/m corresponds to around 250 MV/m peak surface electric field

The high field leads to 'classic' vacuum breakdown. Field emission, neutral copper emission, plasma formation, kA currents, collapse of fields. Beam is kicked, luminosity or brightness lost



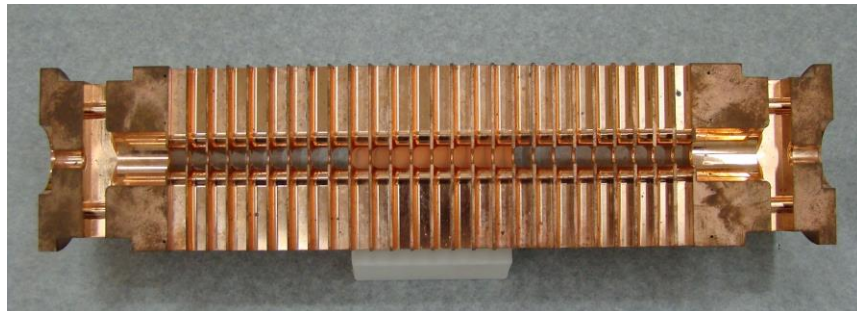
Surface electric field concentration on the beam-aperture irises



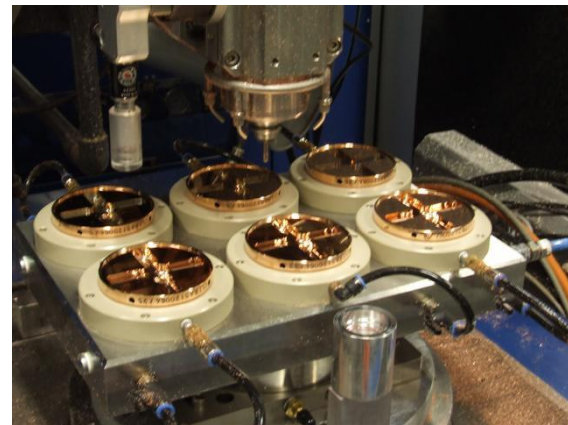
Courtesy of Walter Wuensch et al., CERN



Technological demands for CLIC accelerating structure



Micron-precision turning and milling.



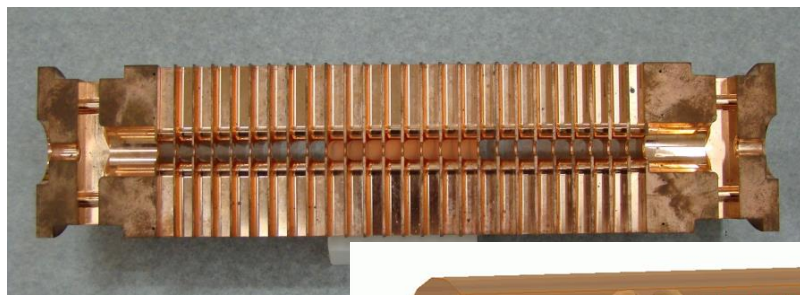
Images are courtesy of CERN collaborators



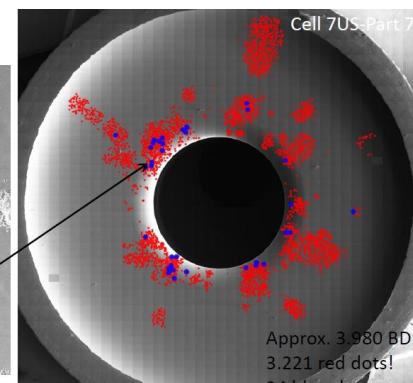
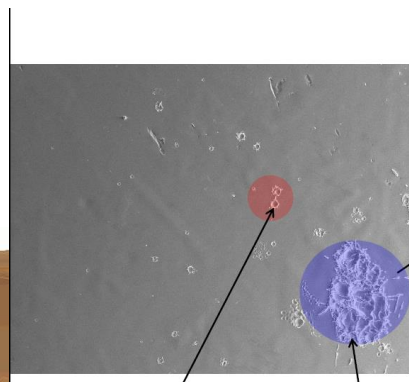
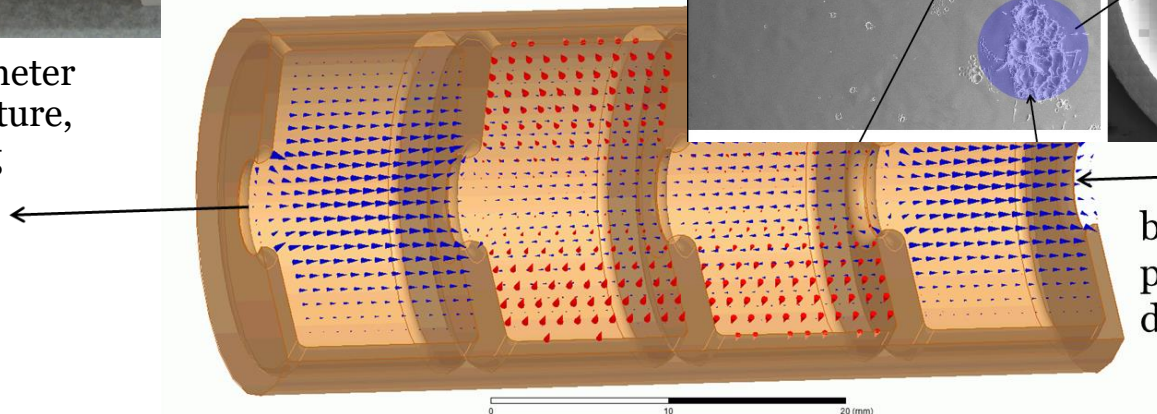
Our activities within CLIC project

We develop the multiscale model to explain the behavior of metal surfaces in extreme condition of accelerating structures.

11.994 GHz X-band



6 mm diameter
beam aperture,
25 cm long

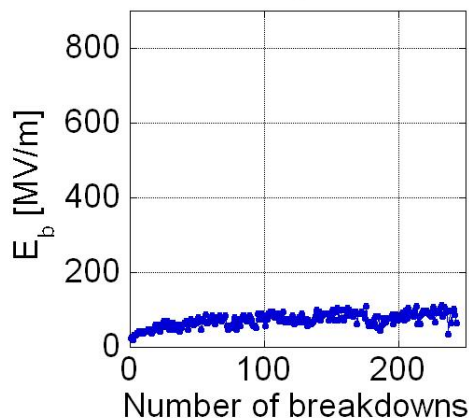


beam
propagation
direction

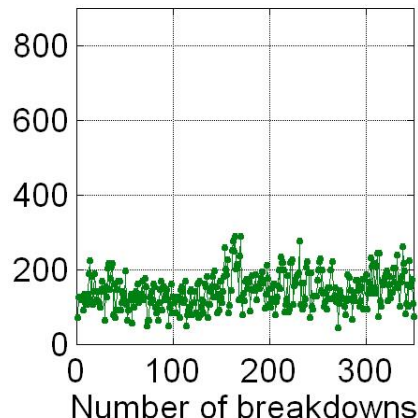


History of tests of different metals: conditioning curves of metals (CERN)

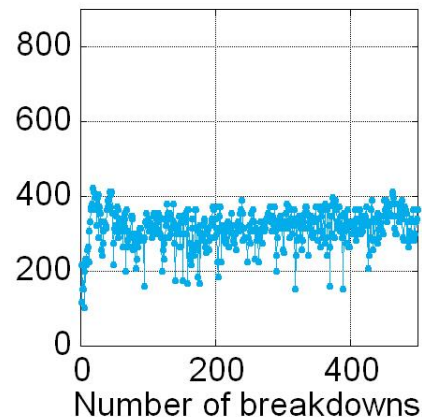
C



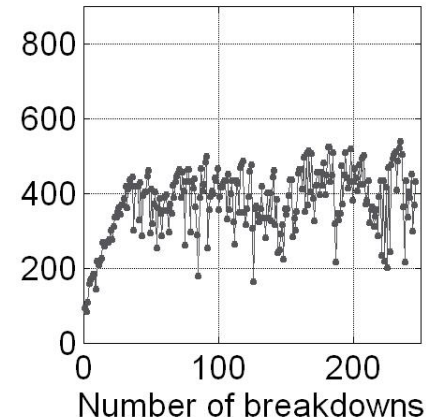
Cu



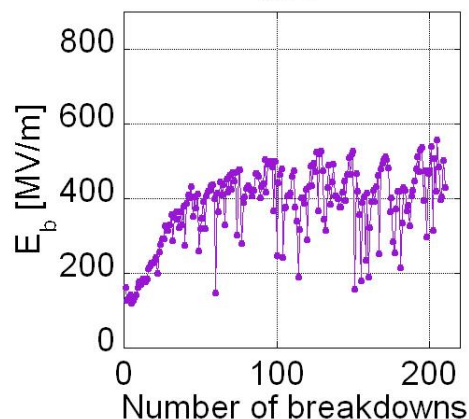
W



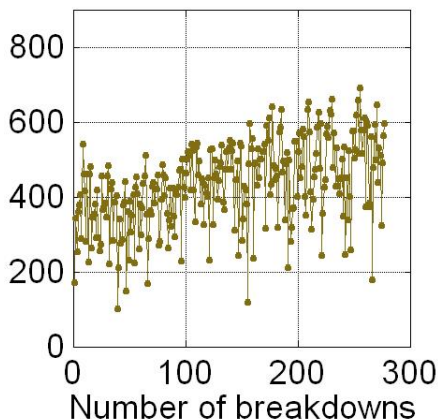
Nb



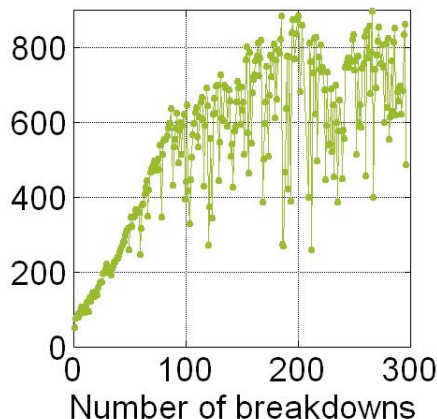
Mo



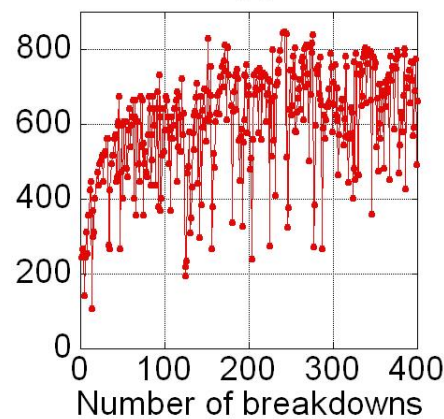
Cr



V



Ti

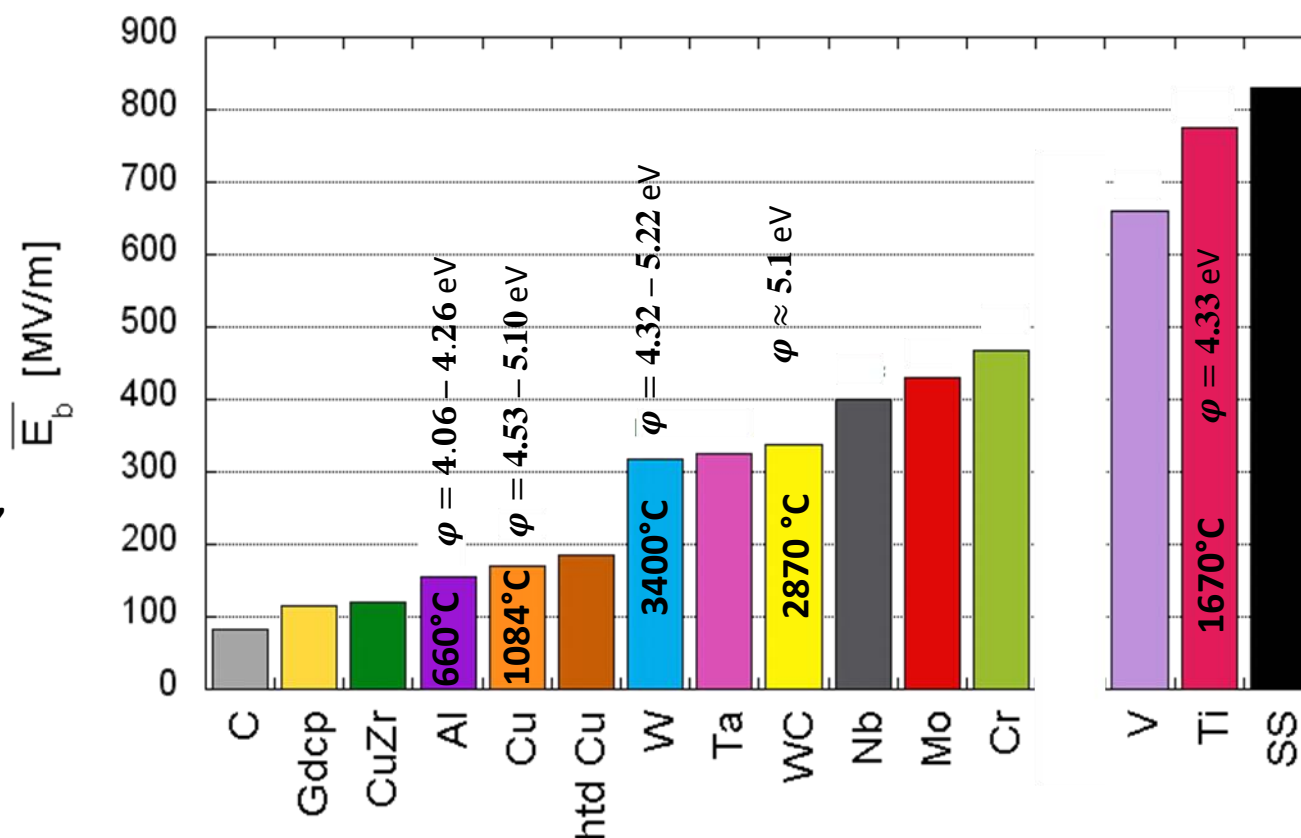


A number of different materials was tested with the purpose of selecting new materials for RF structure fabrication [Descoeudres et al., Phys. Rev. ST Accel. Beams 12, 032001 (2009)]



How lattice structure may play a role

Ranking of the metals with respect to their breakdown resistance did not yield any positive correlation with melting points or surface electronic properties



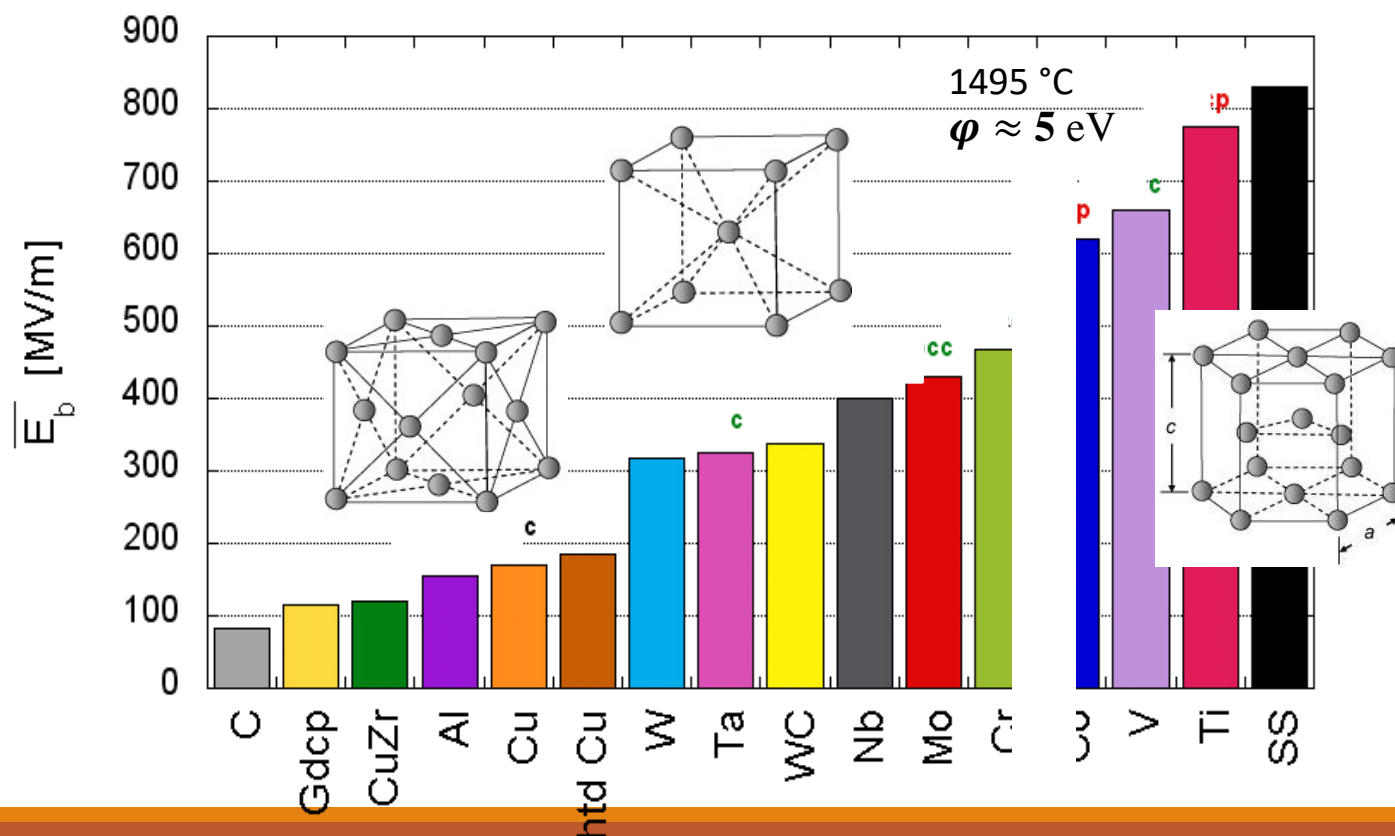
[A. Descoeudres T. Ramsvik, S. Calatroni, M. Taborelli, and W. Wuensch, Phys. Rev. ST Accel. Beams 12, 032001 (2009)]



How lattice structure may play a role

In FCC (face-centered cubic) the dislocation are the most mobile and HCP (hexagonal close-packed) are the hardest for dislocation mobility.

The dislocation activity is strongly bound to the atomic structure of metals, where the periodic crystal structure is prominent.

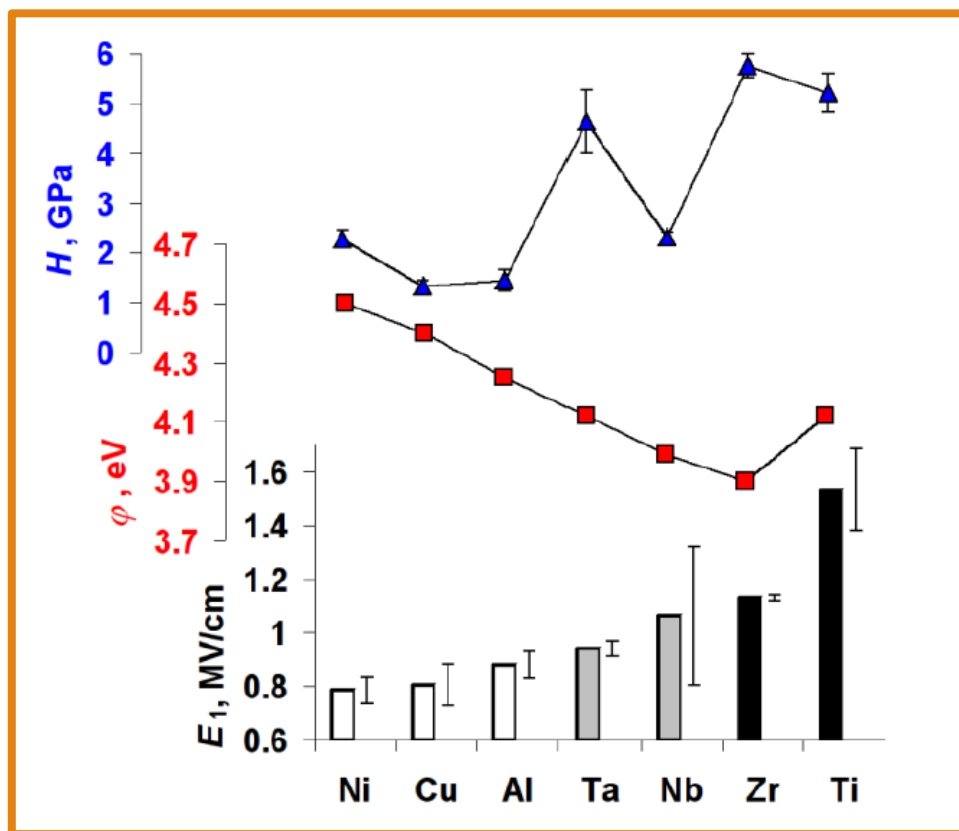


A. Descoeudres, F. Djurabekova, and K. Nordlund, DC Breakdown experiments with cobalt electrodes, CLIC-Note 875, 1 (2010).



Independent study in Tomsk, Russia

Different experiment, different surface treatment, different condition.
The trend is... the same!



Microhardness, electron work function (values recommended in [24]), SPES *E*1, and crystalline structure (empty bars – FCC, half-tone bars – BCC, solid bars – HCP) vs the electrode pair materials

[S.A. Onischenko, A.S. Grenadyorov, K.V. Oskomov, E.V. Nefedtsev and A.V. Batrakov@XXVIIth Int. Symp. on Discharges and Electrical Insulation in Vacuum – Suzhou – 2016]

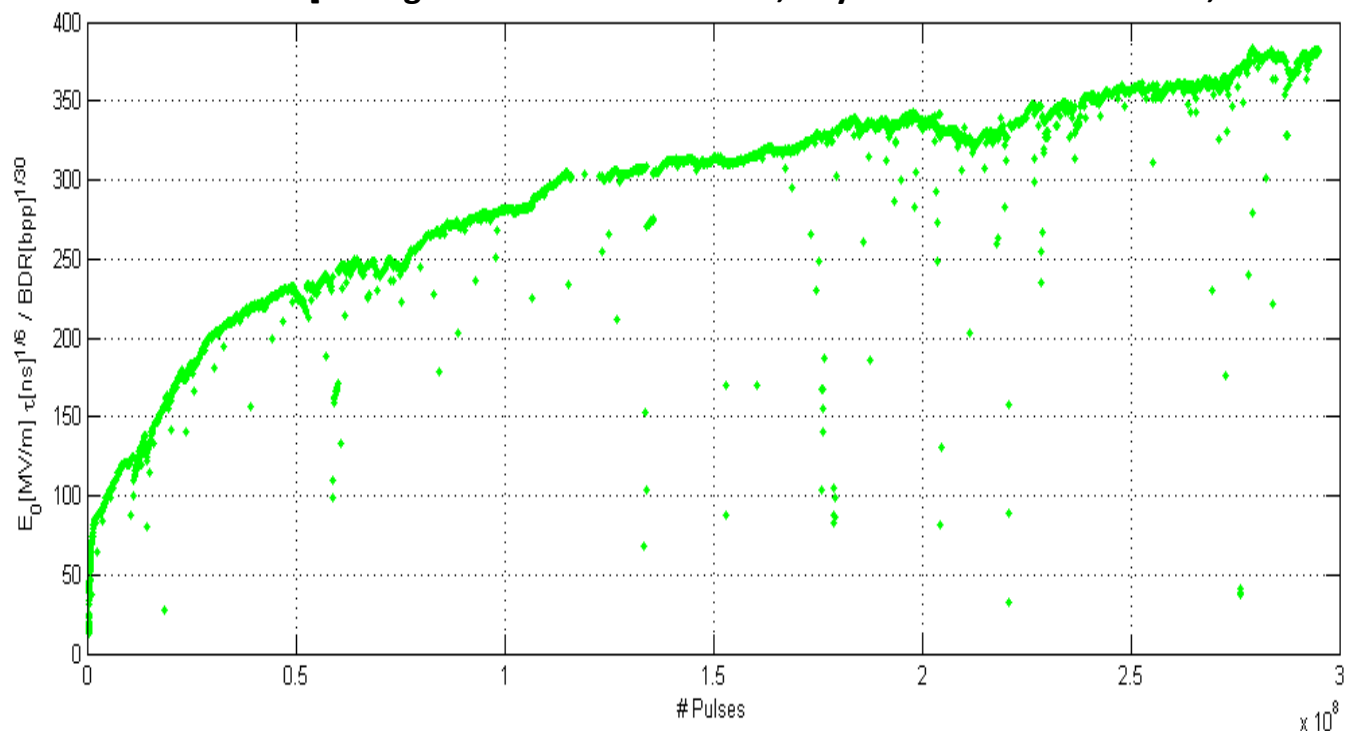


Conditioning history of two structures at KEK and CERN

CERN TD26R05CC conditioning history plot

11 168 BDs

[A. Degiovanni and W.Wuensh, Phys. Rev. Accel. Beams 19, 032001 (2016)].

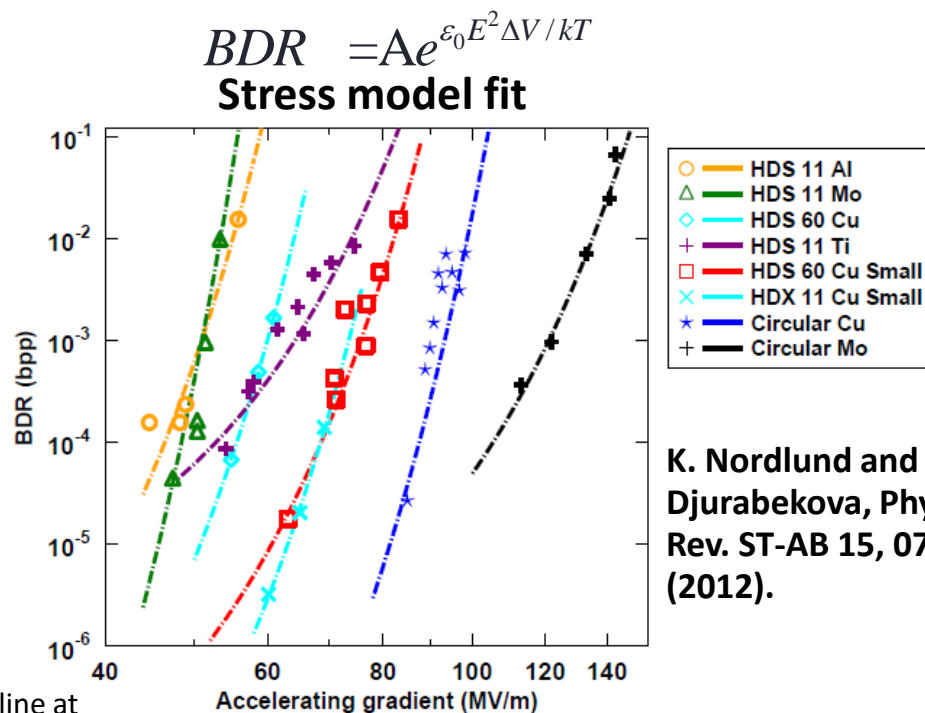
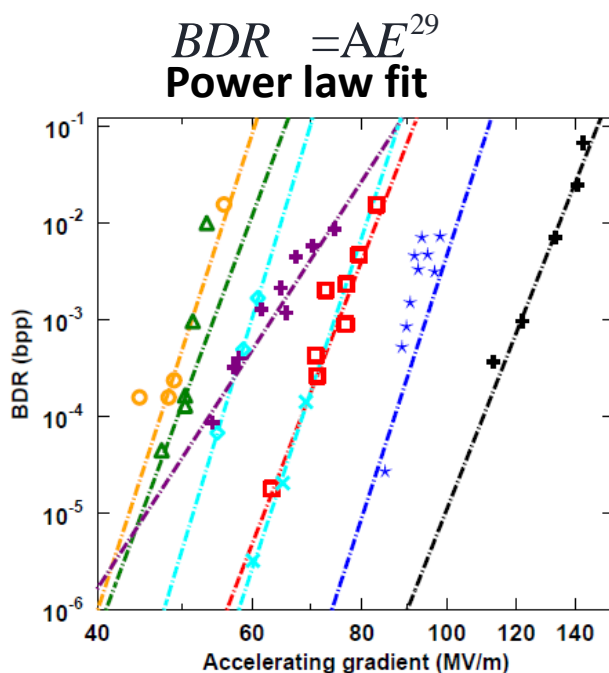


The conditioning behaviour of a CLIC prototype accelerating structure. The time corresponds to over four months of operation at 50 Hz. The vertical scale is the accelerating gradient normalized for pulse length and breakdown rate.



Dislocation-based model for electric field dependence

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



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

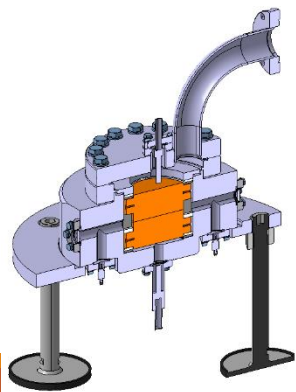
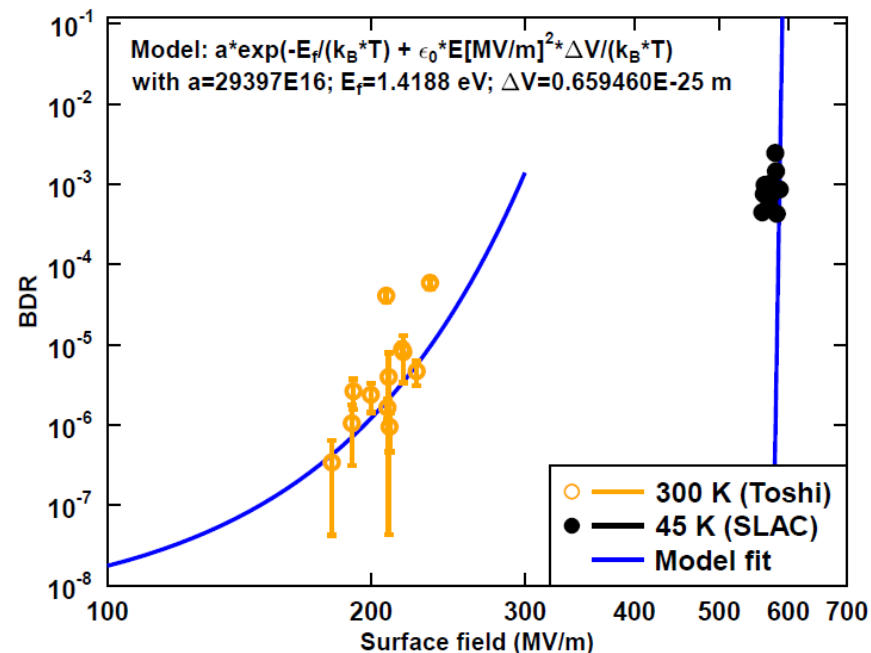
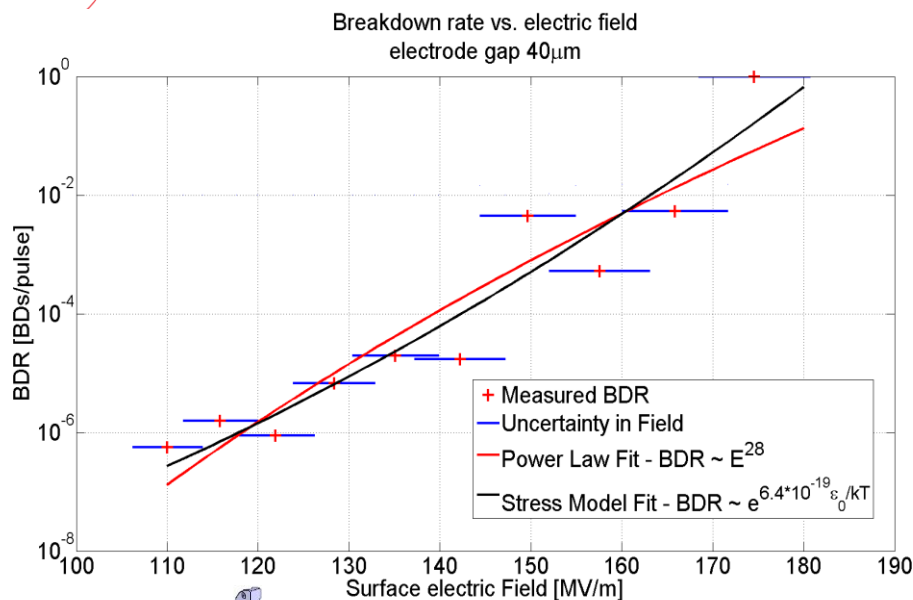
[W. Wuensch, public presentation at the CTF3, available online at <http://indico.cern.ch/conferenceDisplay.py?confId=8831>.] with the model.]

More elaborated model based on consideration of critical density of dislocations was recently suggested in [E. Engelberg, Y. Ashkenazy, M. Assaf, Phys. Rev. Lett. 120, 124801 (2018)]



More data fit to the model

BDR in the pulsed dc (CERN)



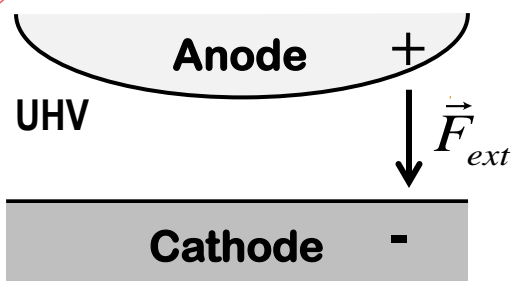
Pulsed DC experiments also give a good agreement with the model.

As a preliminary test, we found that the same fitting parameters can reproduce both data taken from KEK (300K) and SLAC (45K) experiments.



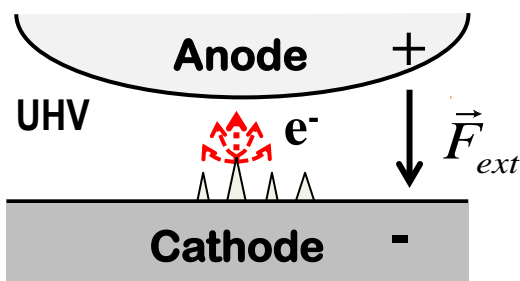
Vacuum arcing model

Stage 1



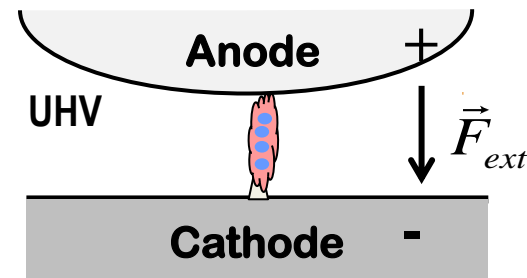
Test system e.g. at CERN; F_{ext} ramps up

Stage 2



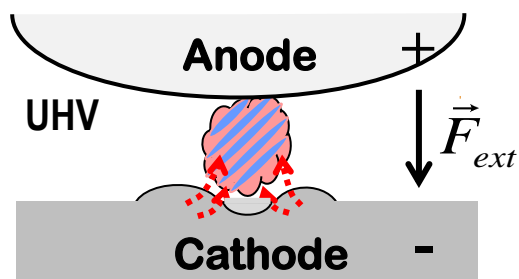
Tips grow on surface (seen as FE currents)

Stage 3



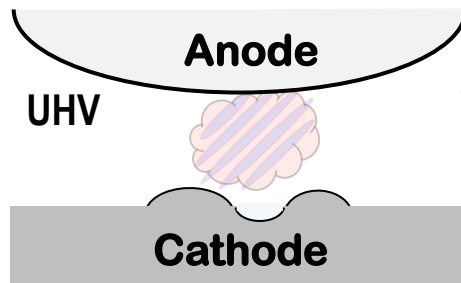
Plasma onset: FE currents, FAE of atoms, tips burn out

Stage 4

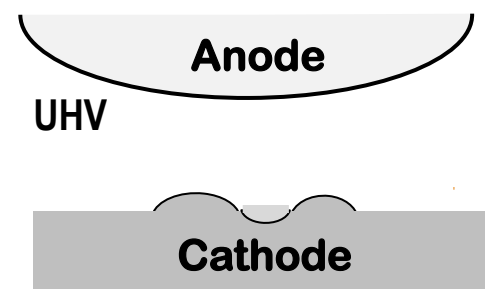


Plasma burning → cathode damage

Stage 5



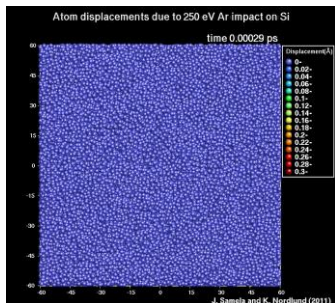
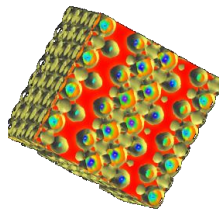
Extinction of energy, plasma burns out



Final damage remains, observed experimentally



Tools in use:



In our group we use all main atomic-level simulation methods:
Density functional theory (DFT)

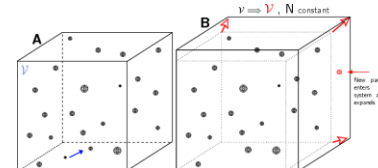
- Solving Schrödinger equation to get electronic structure of atomic system (SIESTA, VASP)

Molecular dynamics (MD)

- Simulation of atom motion, including electric charging effects
- Hybrid ED-MD (HELMOD, FEMOCS) approach

Simulation of atom or defect migration in time

- Kinetic Monte Carlo (KMC)
- Kimocs

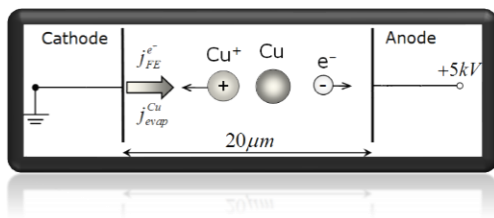


Simulations of plasma-wall interactions

- Arc-PIC

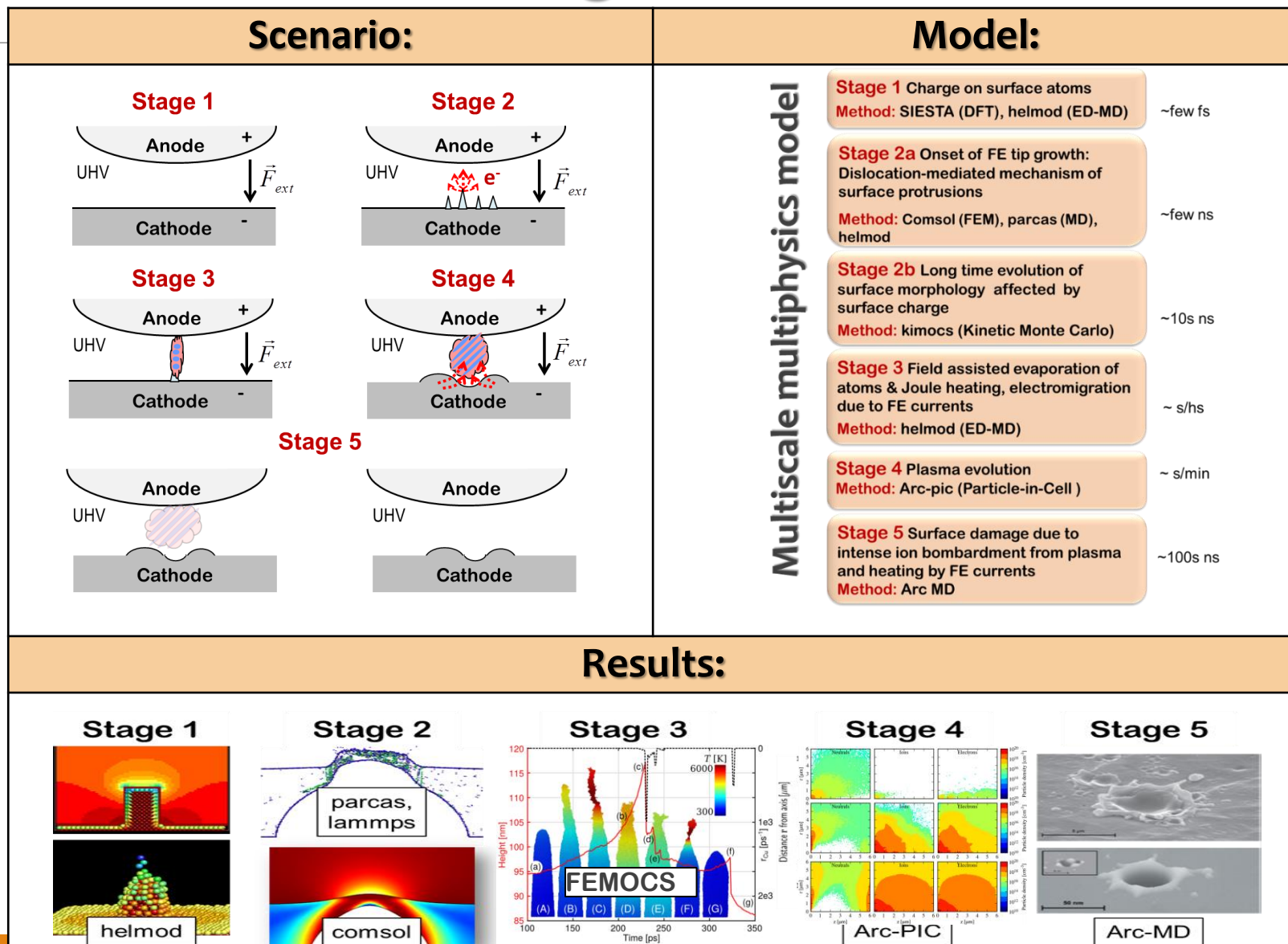
Simulation of plasma particle interactions with surfaces

- Arc-MD (based of PARCAS)



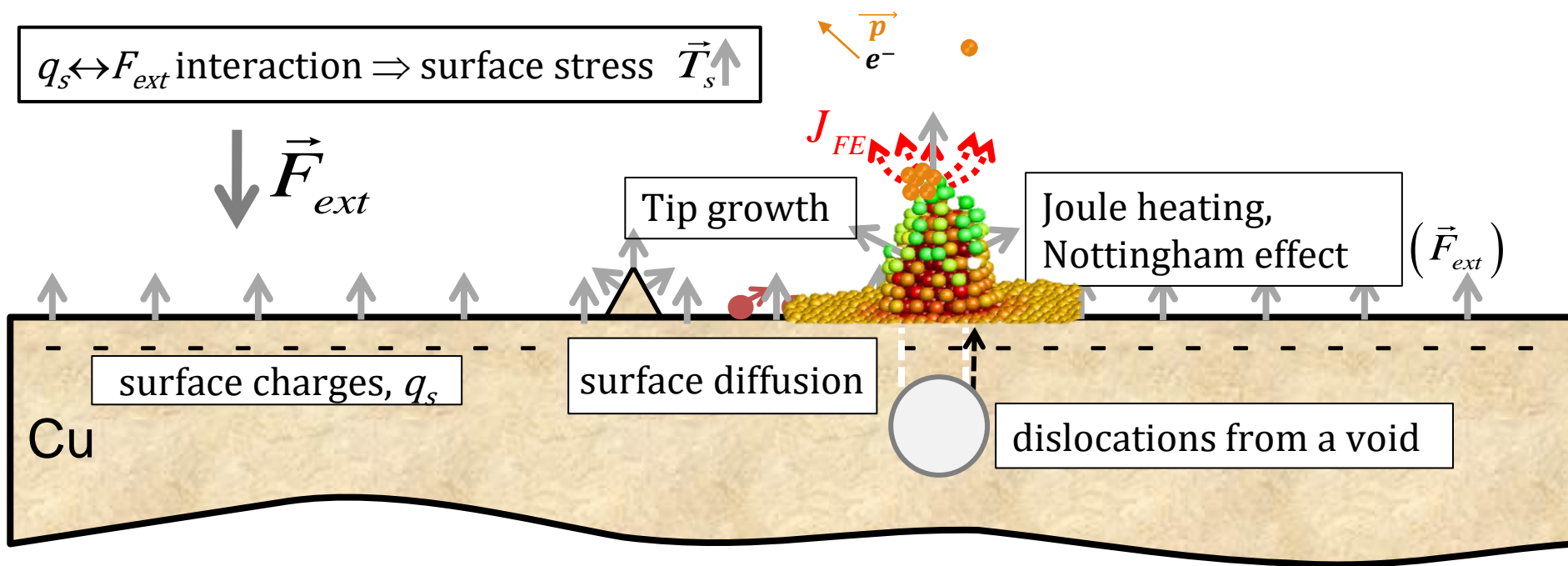


Multiscale modelling of breakdown



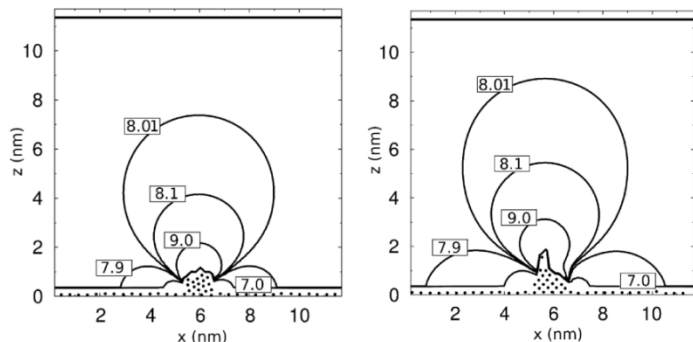
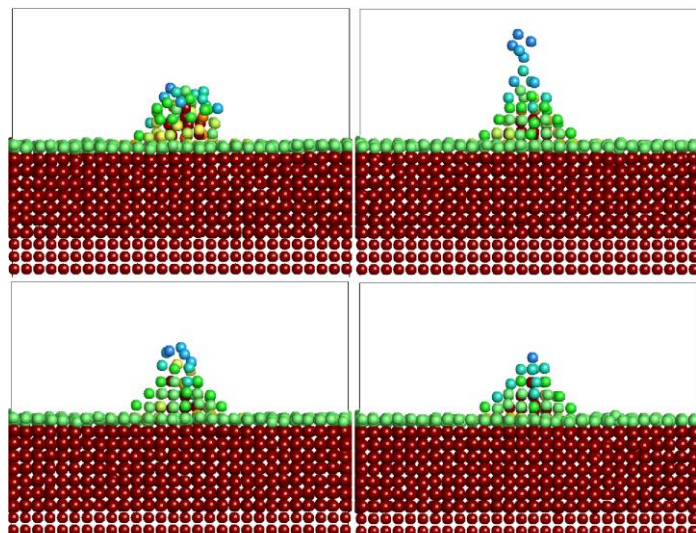


Mechanisms on and under the surface in the presence of electric fields





Electric field effects in MD simulations for Cu surfaces



Initially we developed a *helmod* code (hybrid ED-MD code, based on classical molecular dynamics model) 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

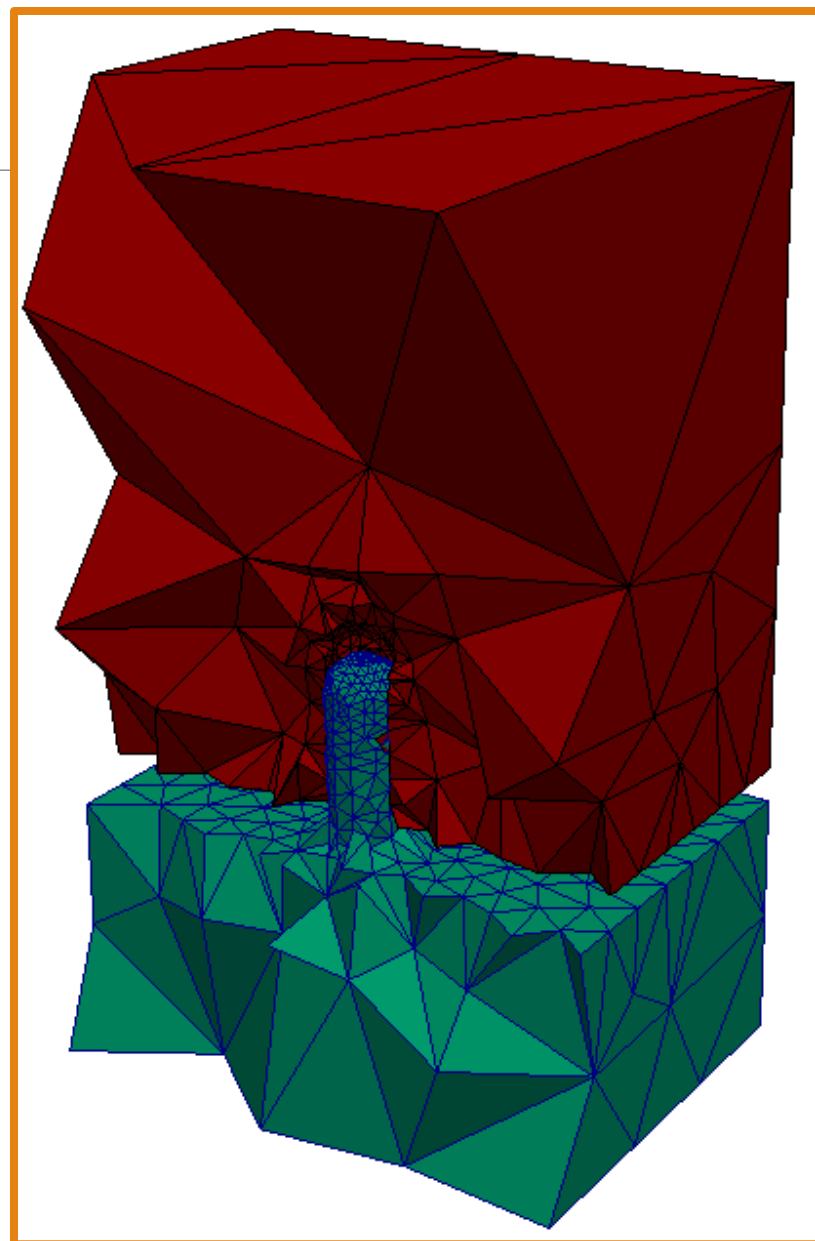
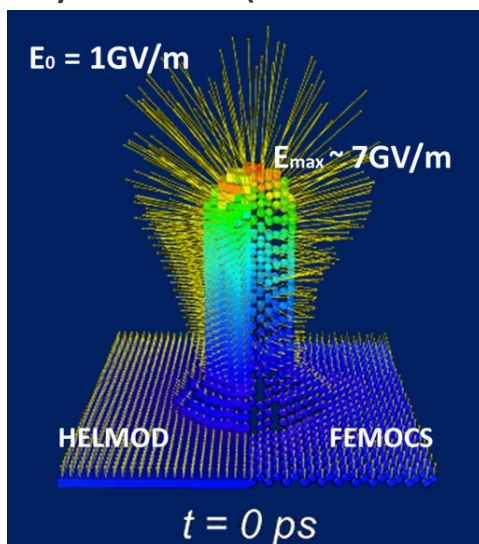
Temperature on the surface tips is sufficient => atom evaporation enhanced by the field can supply neutrals to build up the plasma densities above surface.

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



Flexible grid to calculate electric field

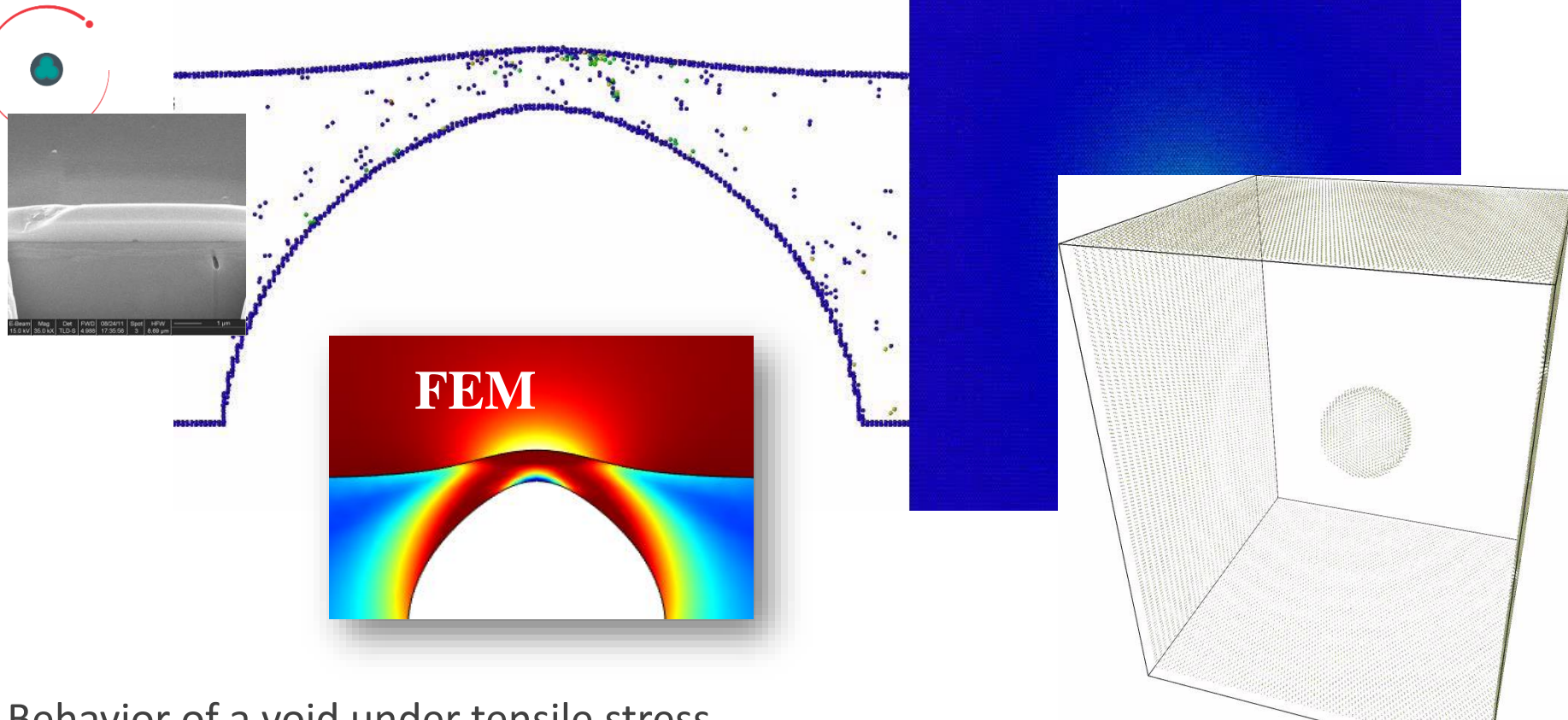
We now have an improved implementation of electric field in MD by using FEM elements. The *Femocs* calculations are more flexible and can reach large scales. More details will be given later on by Andreas Kyritsakis (now Uni.of Tartu)



(By Mihkel Veske)



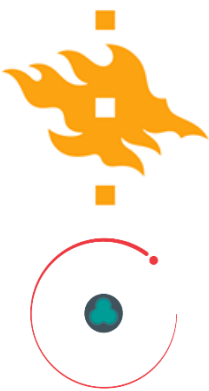
MD simulation of plastic activity under a high electric field



Behavior of a void under tensile stress due to an electric field (Simulations are done with the *helmod* code)

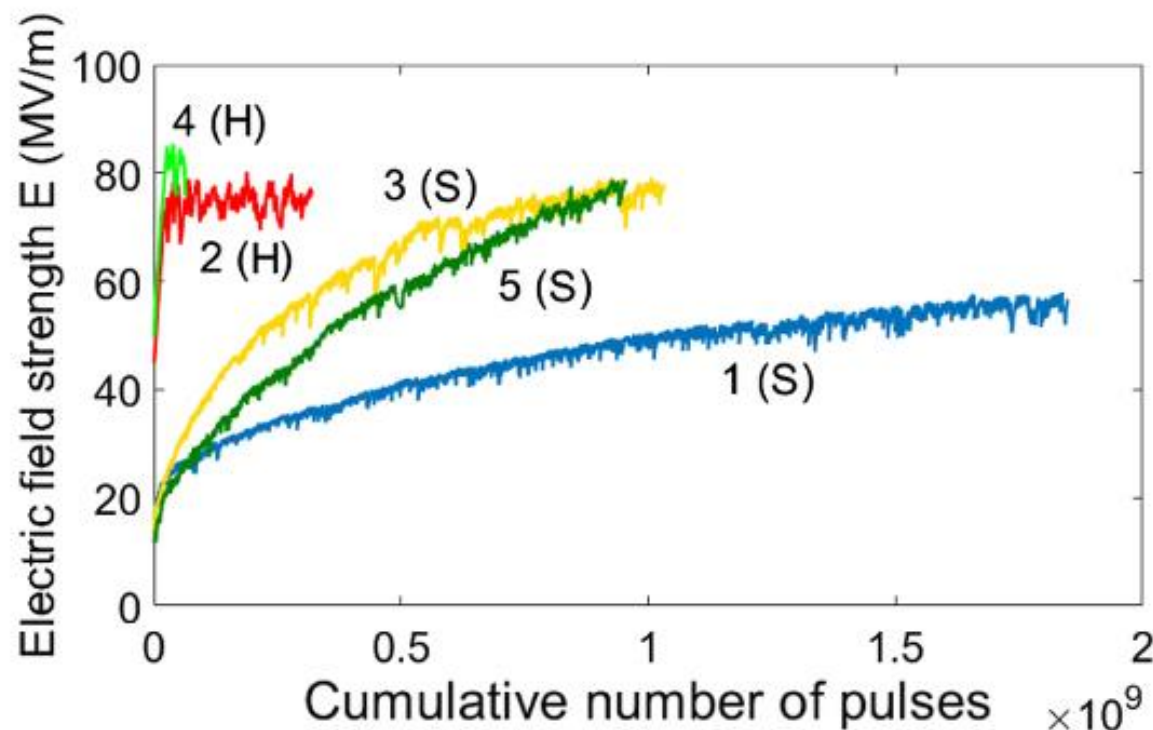
MD in [A. S. Pohjonen, S. Parviainen, T. Muranaka, and F. Djurabekova, JAP 114, 033519 (2013)]

FEM in V. Zadin, A. Pohjonen, A. Aabloo, K. Nordlund, and F. Djurabekova, Phys. Rev. ST-AB (2014),



Confirmation of dislocation-mediated mechanisms

Recently we showed experimentally that "soft" (S) copper (strongly annealed in a thorough thermal cycle) conditions much slower than the "hard" (H) copper (as-prepared machine-turned sample) [A. Korsbäck et al., Phys. Rev. Accel. Beams 23,033102 (2020)]



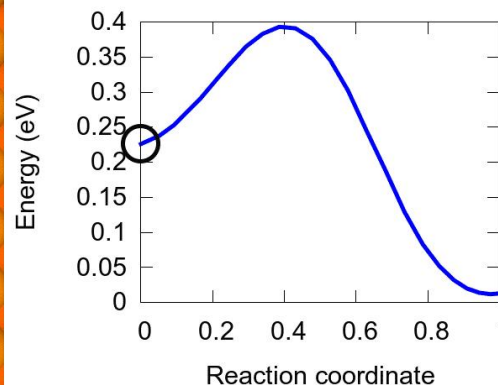
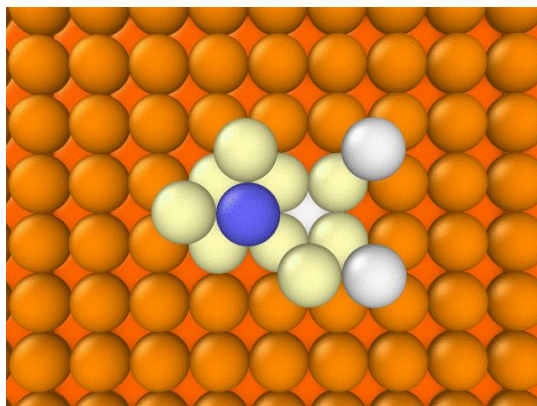


Surface diffusion model

We simulate the surface diffusion using kinetic Monte Carlo method. In this method, the evolution of system proceeds via diffusional jumps which are thermally activated and selected among all the available jumps according the probability

$$\Gamma = \nu_D \exp\left(-\frac{E_b}{k_B T}\right)$$

k_B and T are Boltzmann constant and substrate temperature, ν_D is the attempt frequency, often approximated by Debye frequency and E_b is the main defining parameter, which shows the change of the Hamiltonian in the initial and the saddle point position.





Surface diffusion in electric fields

Adatoms in electric fields become polarized.

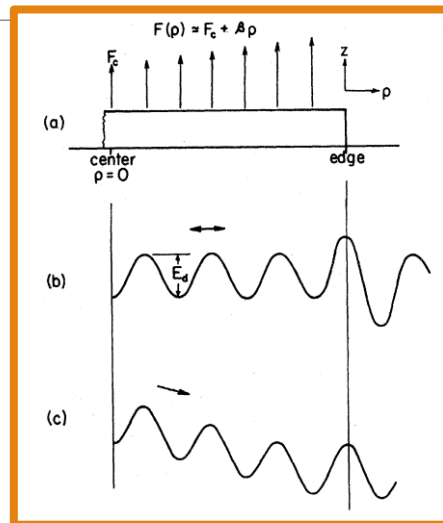
This introduces a dipole moment, which experience the force in the direction perpendicular to the field, that will bias the adatoms migration towards stronger fields

We have implemented this field effect into our Kinetic Monte Carlo (KMC) code Kimocs, which was developed to simulate the surface diffusion

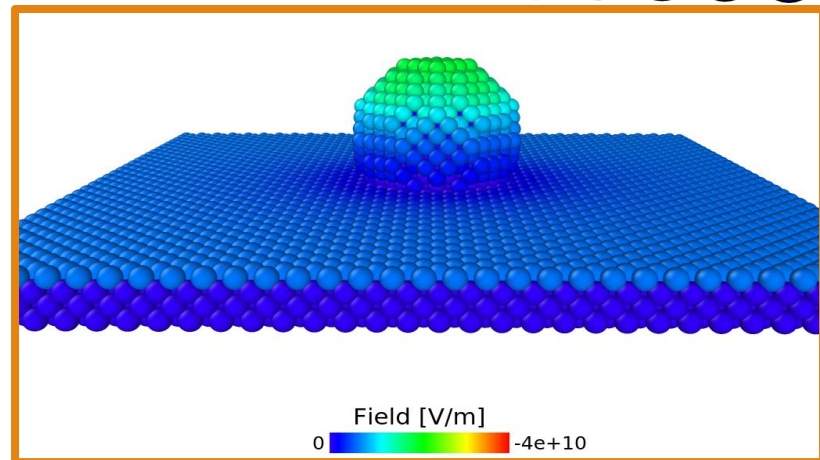
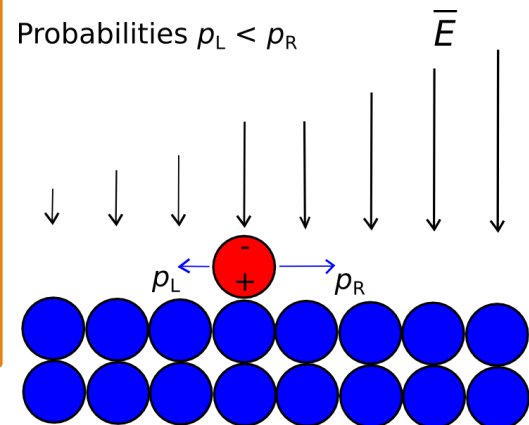
Directional walk is achieved by thermal activations and taking into account the reduction in potential energy.

$$\Delta E(F) = E(0) - E(F) = \mu_t \Delta F + F_t \Delta \mu + \alpha_t F_t \Delta F + \frac{1}{2}(\Delta \alpha) F_t^2$$

μ and α are the dipole moment and polarizability of the adatom



[Tsong & Kellogg PRB 1975]



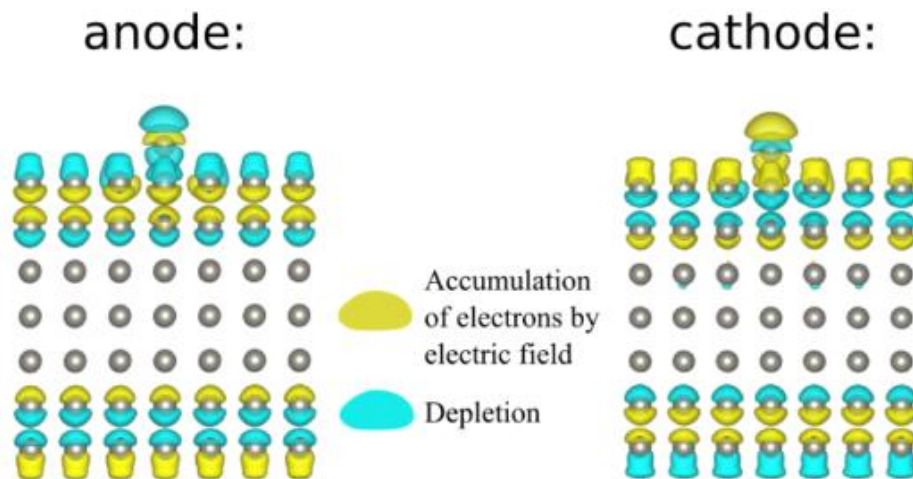


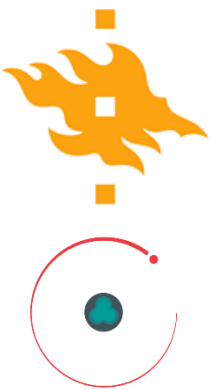
Surface diffusion in electric fields

Growth mechanism of Cu tips (V. Jansson)

The effect of electric field was taken into account by using the Tsong's model of surface adatoms dipoles. We improved the original understanding of the dipole moments and polarizability from the first principles, using density functional theory calculations (details are in [A. Kyritsakis et al ., Phys. Rev. B 99, 205418 (2019)]). The new barriers are estimated as $E_b = E_b^0 + \Delta E_{\text{dipole}}(\mu_{\text{sys}}, \alpha_{\text{sys}}, \mathbf{F})$

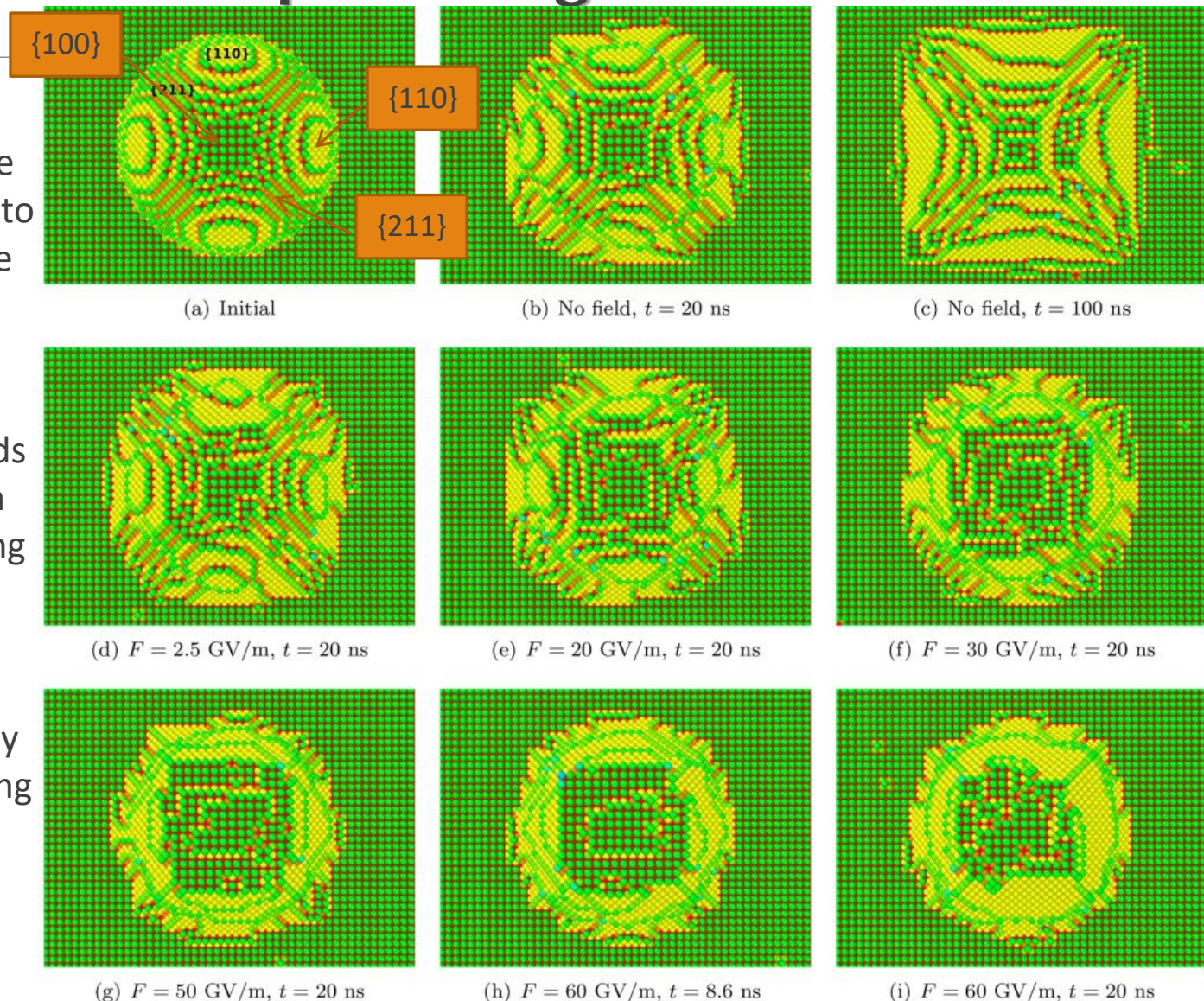
The new values enabled to perform more realistic simulations of surface diffusion under high electric fields





Evolution of W tip under high electric fields

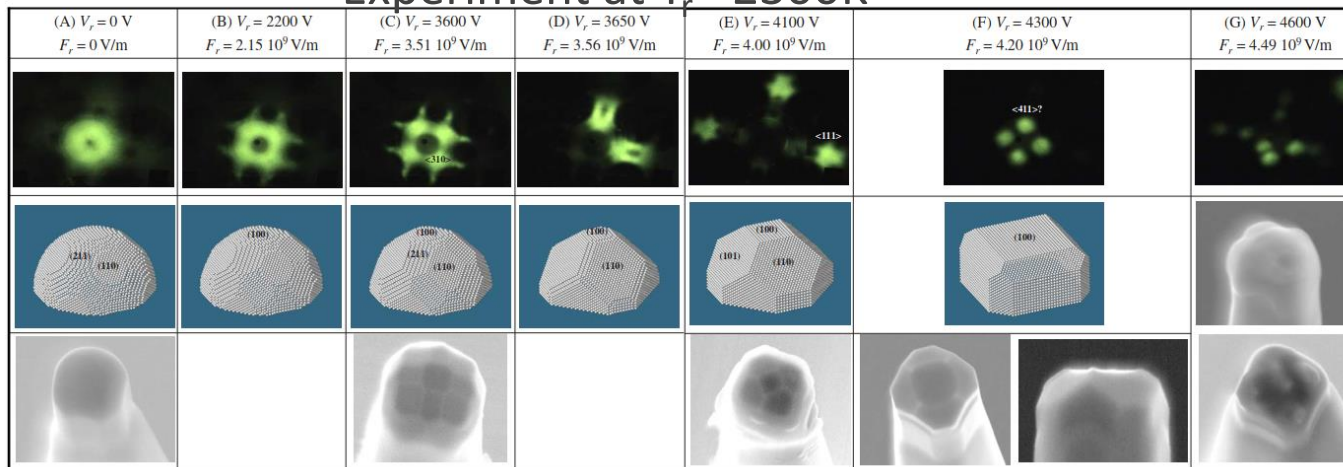
We used the new model to simulate the surface relaxation under high electric fields on tungsten tip, assuming the same value of dipole and polarizability for all moving adatoms





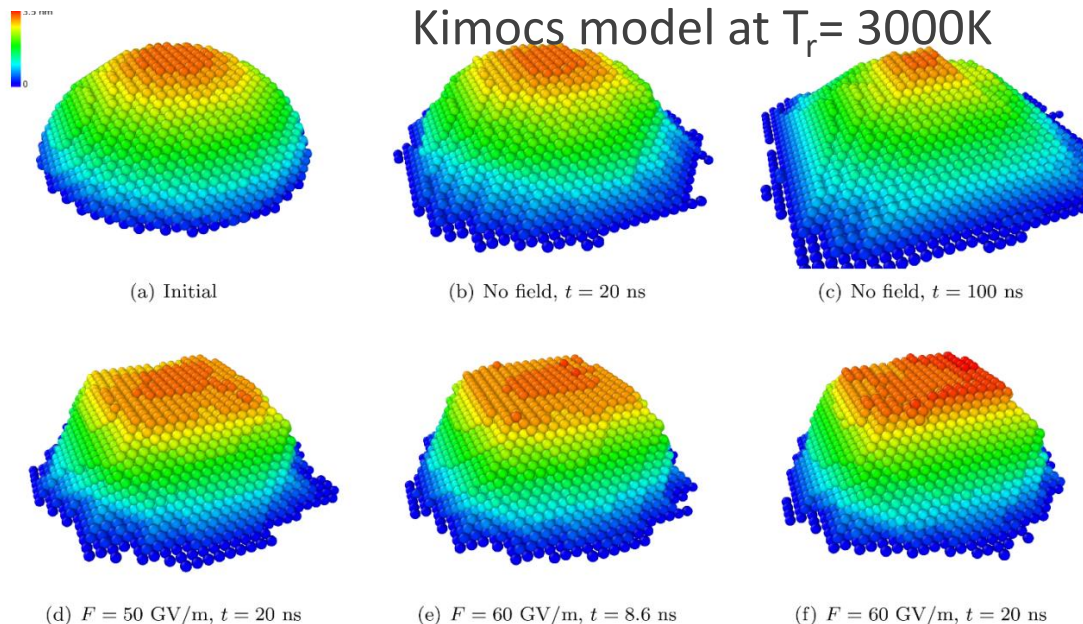
Comparison versus experiment

Experiment at $T_r = 2300\text{K}$



S. Fujita and H. Shimoyama,
Phys. Rev. B 75
(2007) 235431

Kimocs model at $T_r = 3000\text{K}$

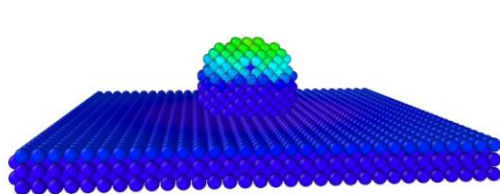


V. Jansson et al.,
Nanotechnology 31 (2020)
355301

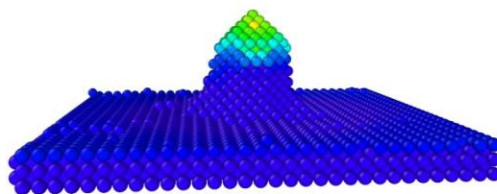


Growth of a nanotip under high electric field

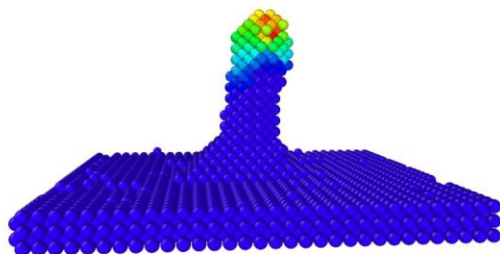
We have also performed the simulations of tip evolution on $\{110\}$ W surface at the applied field of 50 GV/m, the temperature of the substrate is 3000 K.



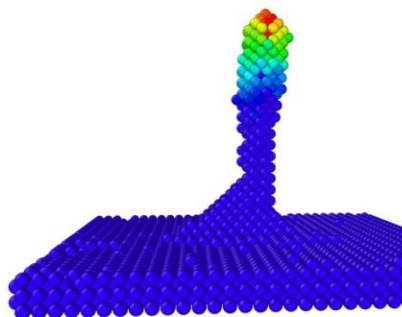
(a) $t = 0$



(b) $t = 2.0$ ns

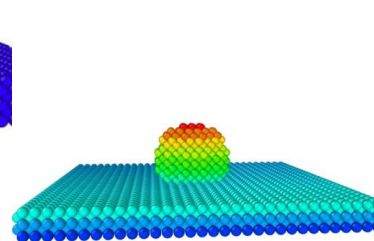


(c) $t = 5.0$ ns

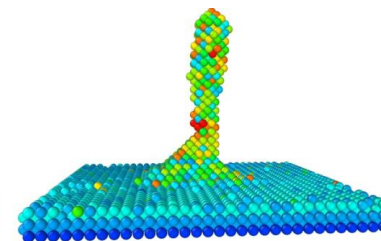


(d) $t = 7.6$ ns

Following the origin of the atoms, we see a strong mixing of due to diffusional jumps affected by the field gradient.



(a) $t = 0$



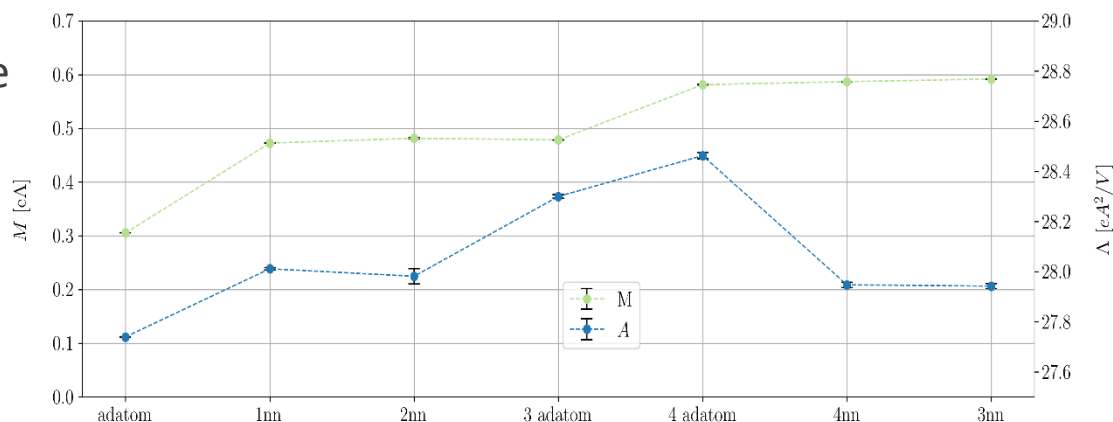
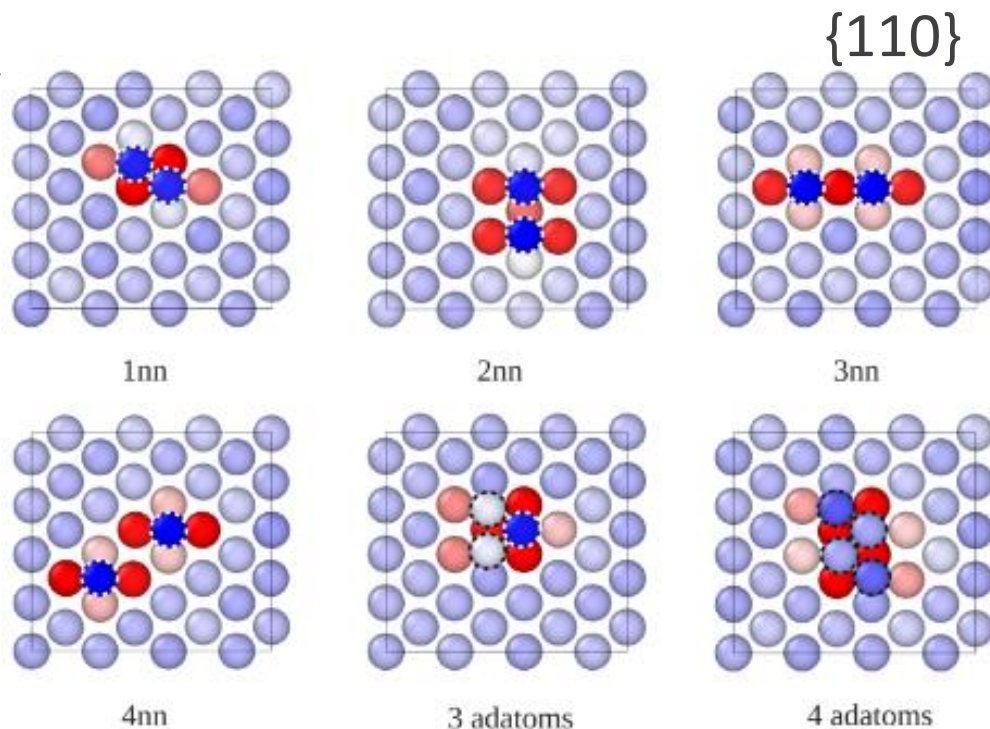
(b) $t = 7.6$ ns



Dipole moments and polarizability of adatom clusters

More detailed analysis of the system with more than one adatom showed that, in principle, the dipole moments and polarizability may differ from the one found for a single adatom due to the overshadowing effect.

- Color is the partial charge estimated by Bader analysis from VASP DFT calculations





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Conclusions

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 and links the breakdown probability with the dislocation activities under the surface

Moreover, we model migration of atoms on the surface

We showed that polarizability characteristics are based on dipole moments due to partial charges accumulated/depleted on the adatoms themselves, but also the charge changes around them

We see promising results towards the surface diffusion driven by the field gradients, but more work needs to be done to build up an accurate model