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HIP

Multiscale modelling of electrical breakdown at high electric field

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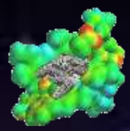
Why do we want to know?



- Since the stone age sparks and arcs in shape of lightning were around. Frightening the human kind they eventually gave a spark for the evolution. People learned to make use of the sparks…
- The application of sparks grew, When the electric field came into play, the short sparks and long maintained arcs could start their inestimable service.
- But, as in ancient days, the question we ask ourselves:

How does all start?

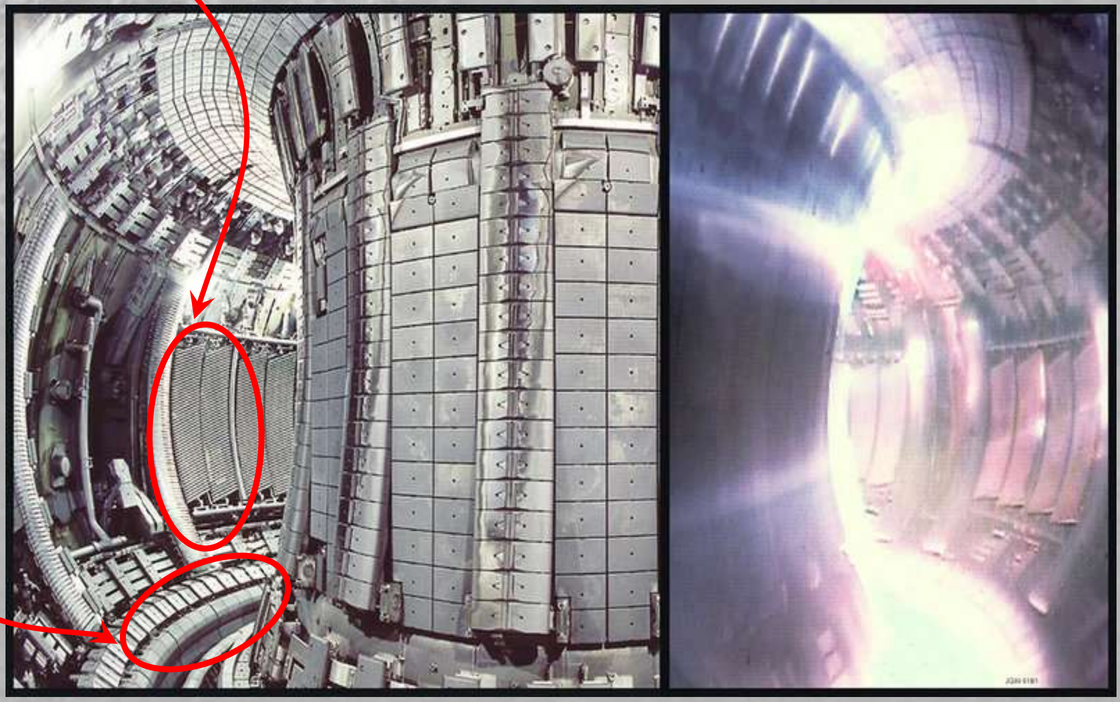
Outline

- Motivation: Multy-km task by atomistic simulations?
- Multiscale model to approach the problem of electrical breakdown
  - Plasma onset due to the external electric field
  - Plasma simulation
  - Surface cratering
- Summary

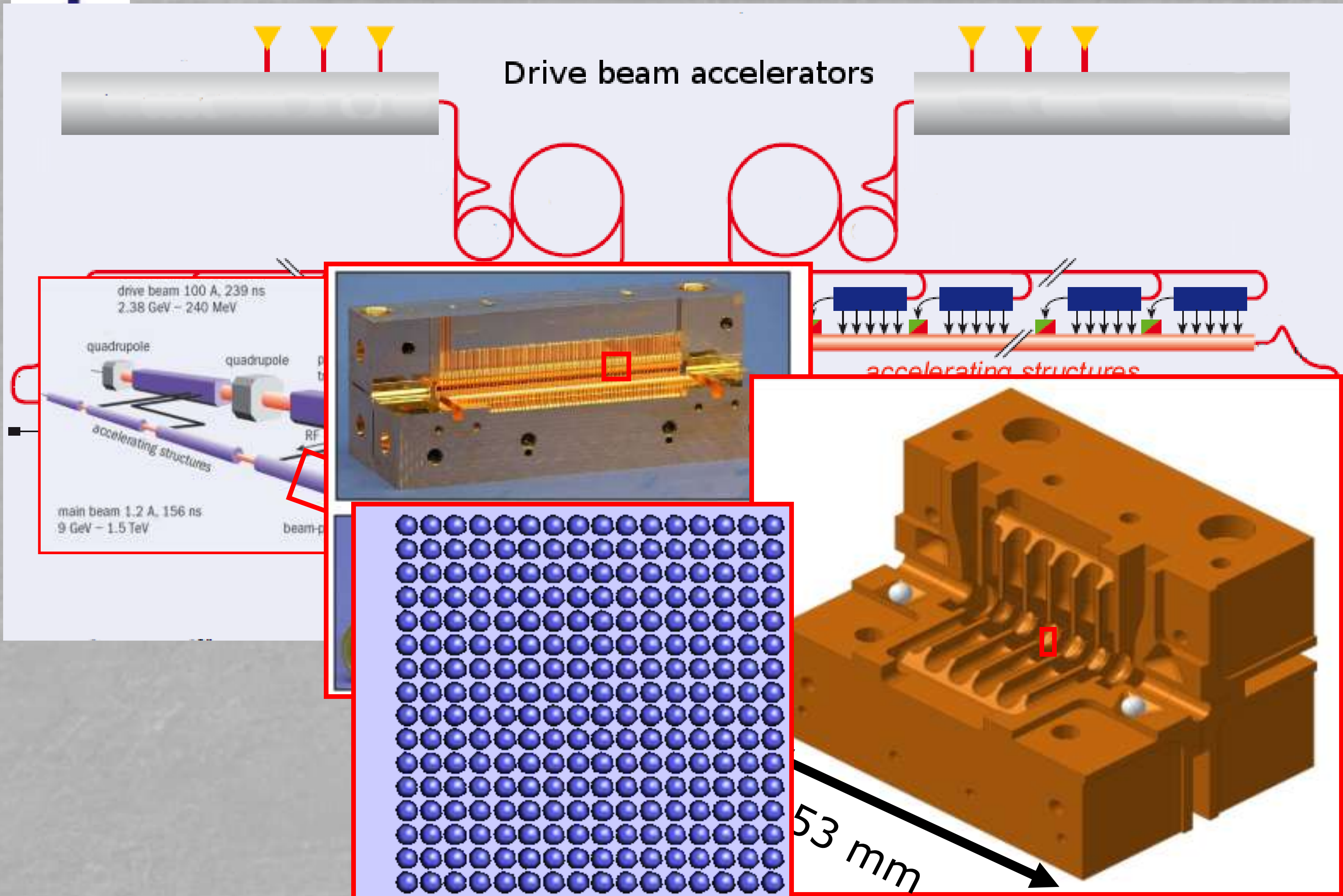
Future of energy supply suffers from tiny problems

- Arcing occurs in fusion reactors:
  - in regions in direct contact with the plasma such as the divertor
  - in region not in direct contact with the plasma such as the limiters

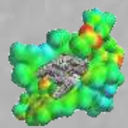
Arc is a significant source of erosion of first wall material and has even been reported to remove limiter coating layers entirely!
Matter flying from the wall into the plasma in an arc can disrupt the normal operation

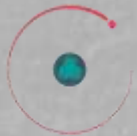


CLIC: "Compact" Linear Collider…

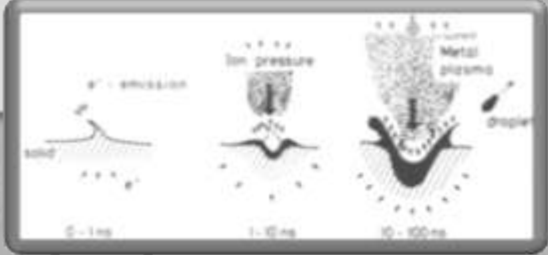


Multiscale model to simulate electrical breakdown





R. Behrisch, Plenum, 1986



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, Molecular Statics.

Stage 3b: Evolution of surface morphology due to the given charge distribution
Method: Kinetic Monte Carlo

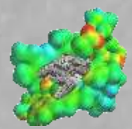
Stage 4: Plasma evolution, burning of arc
Method: Particle-in-Cell (PIC)

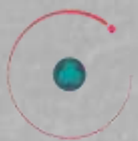
~10s ns

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

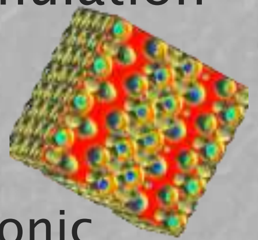
~

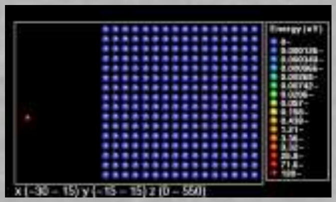
Tools in use:



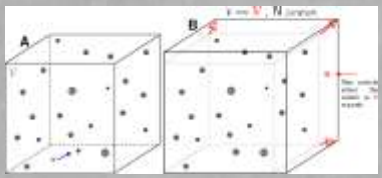


- In our group we use all main atomic-level simulation methods:
  - Density functional theory (DFT)
    - Solving Schrödinger equation to get electronic structure of atomic system





  - Molecular dynamics (MD)
    - Simulation of atom motion, classically and by DFT



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

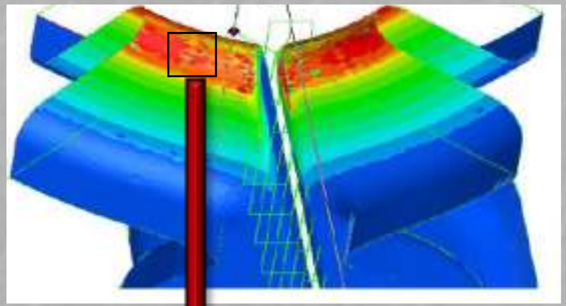
  - Simulations of plasma-wall interactions
    - Simulation of plasma particle interactions with surfaces
- We use all of them to tackle the arcing effects!

External electric field in MD simulations

Macroscopic field to…

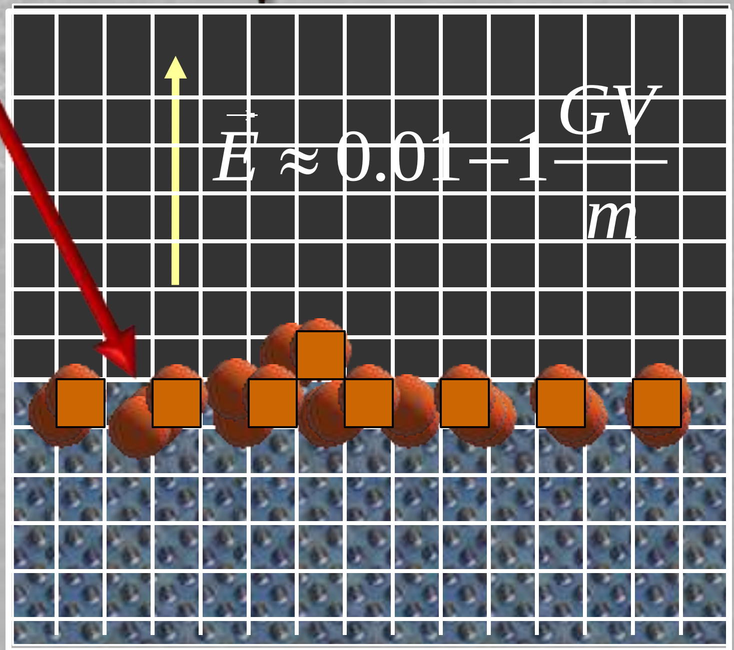
- Gauss law by 'pllbox' technique

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

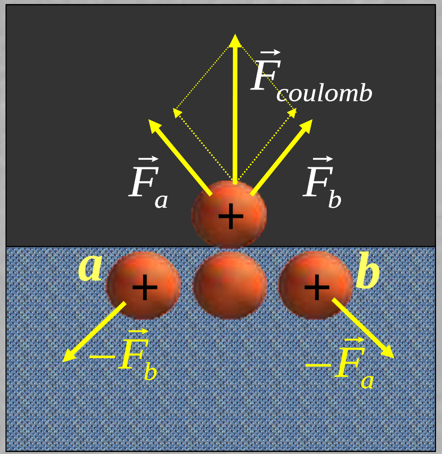


Due to the external electric field the surface attains charge

…the atomic level:



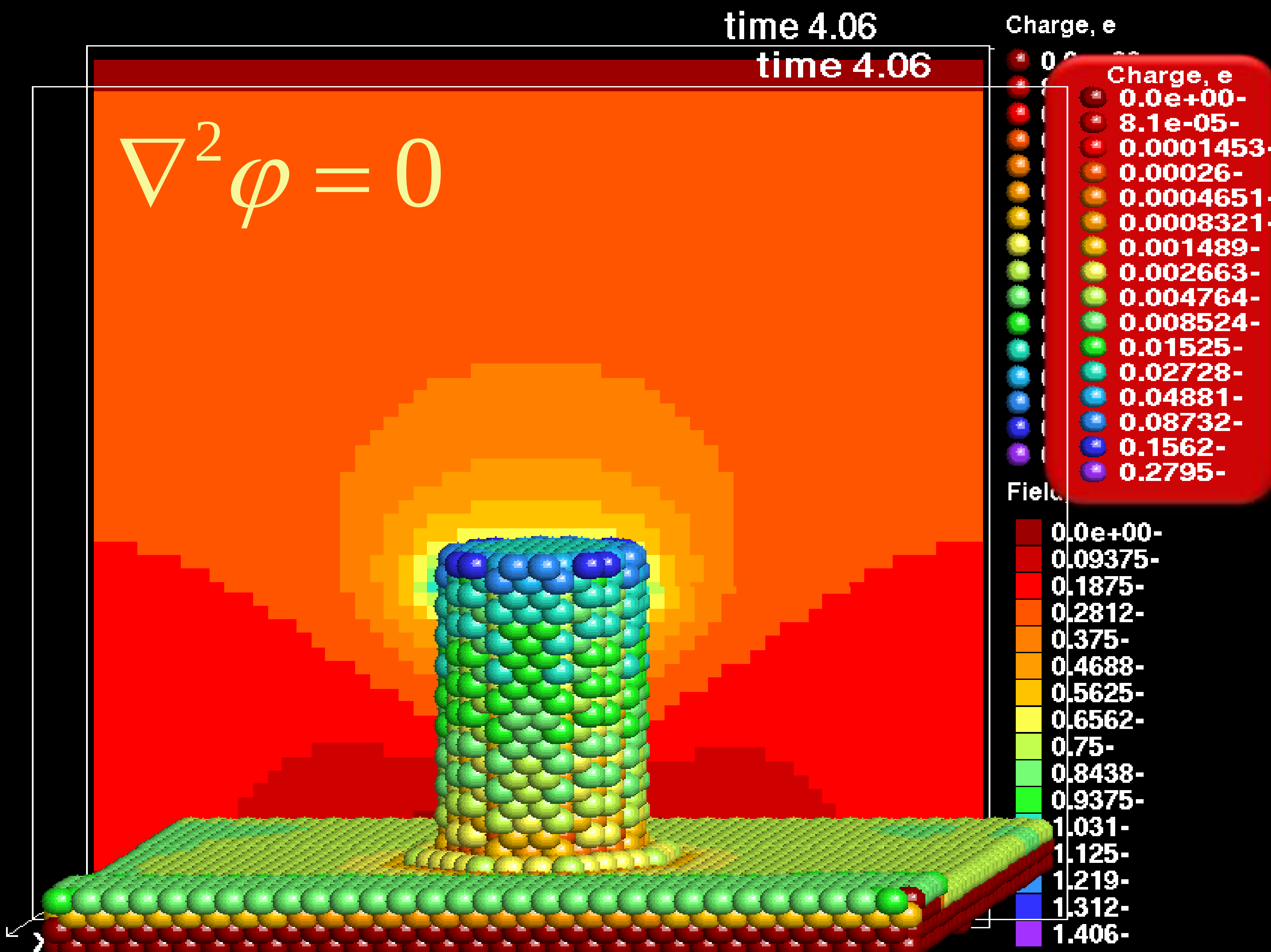
Two electric forces modify the motion of charged atoms:



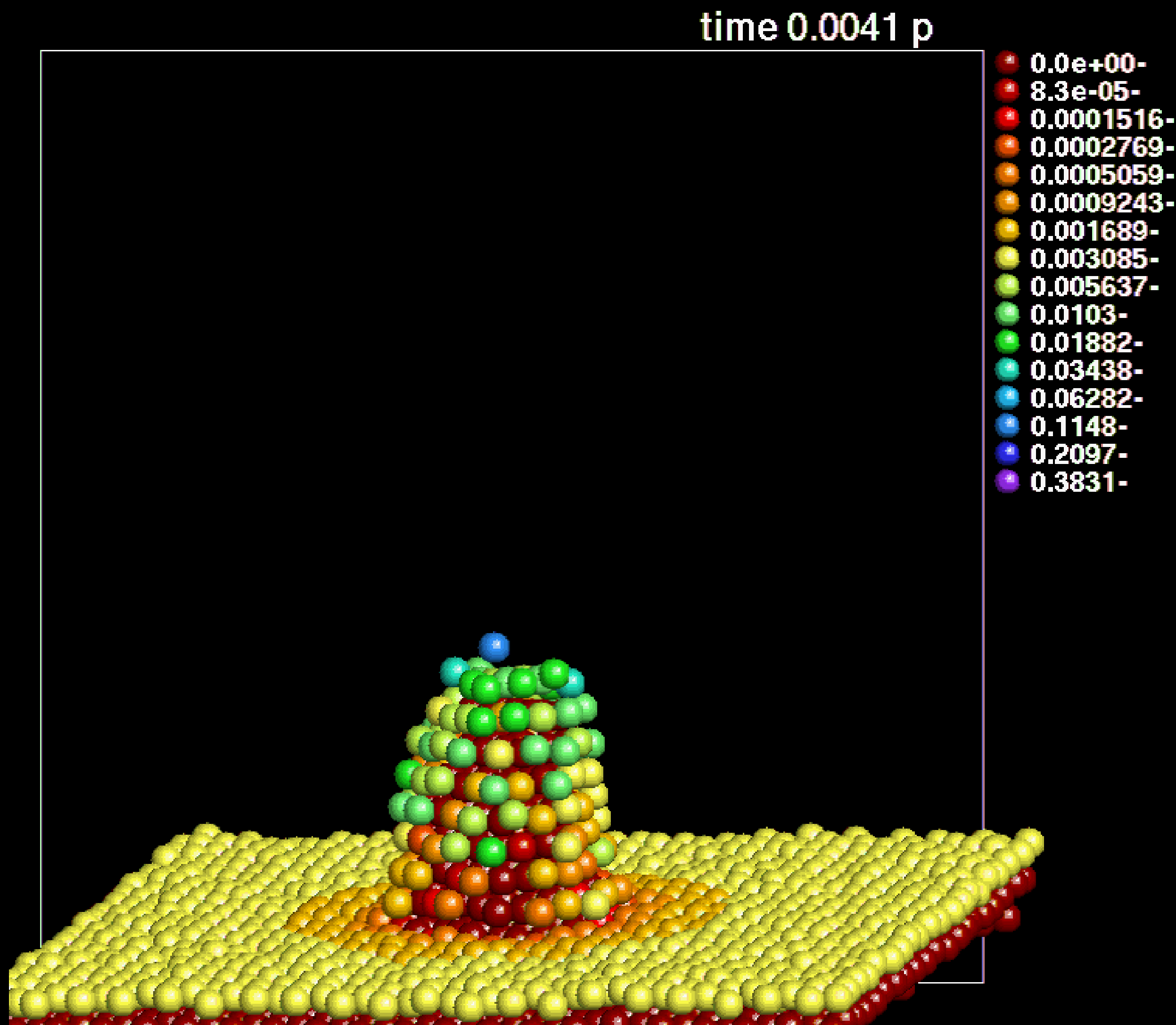
$$\vec{F}_L = \vec{E}q$$

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

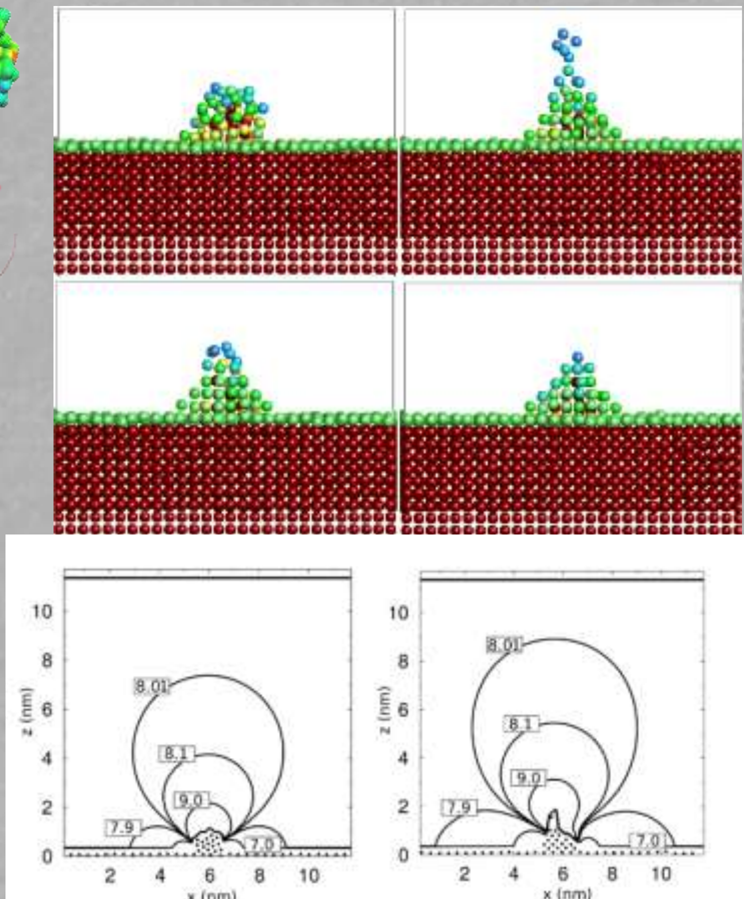
Solution of 3d Laplace equation for the surface with the tip of 20 atomic layers, mixed boundary condition (color represents the charges)



Atom/cluster evaporation from Cu(100) @ 500 K, $E_0 \sim 1$ GV/m



Evolution of a tip placed on Cu surface

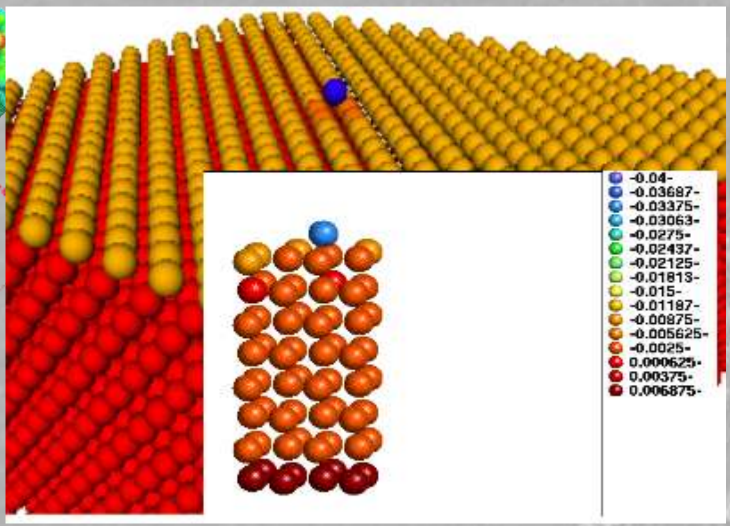


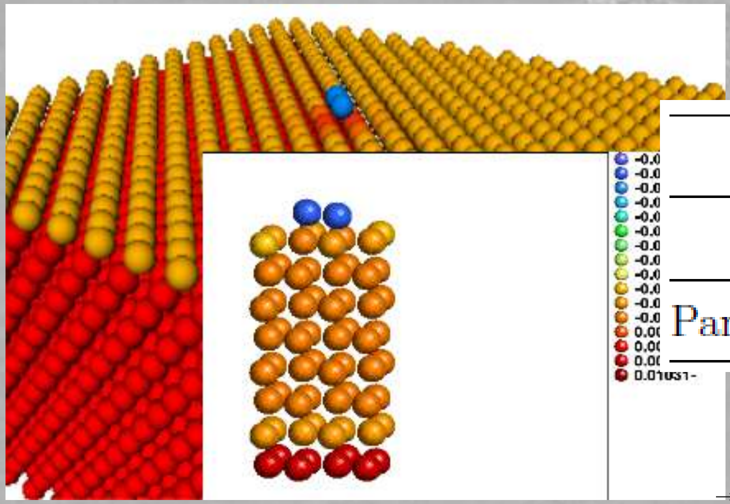
F. Djurabekova, S. Parviainen, A. Pohjonen and K. Nordlund, PRE 83, 026704 (2011).

- Follow evolution of the surfaces by calculating the partial charge induced on metal surface atoms
- The dynamics of atom charges follows the shape of electric field distortion on tips on the surface
- Temperature of the surface 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_o=-1 GV/m



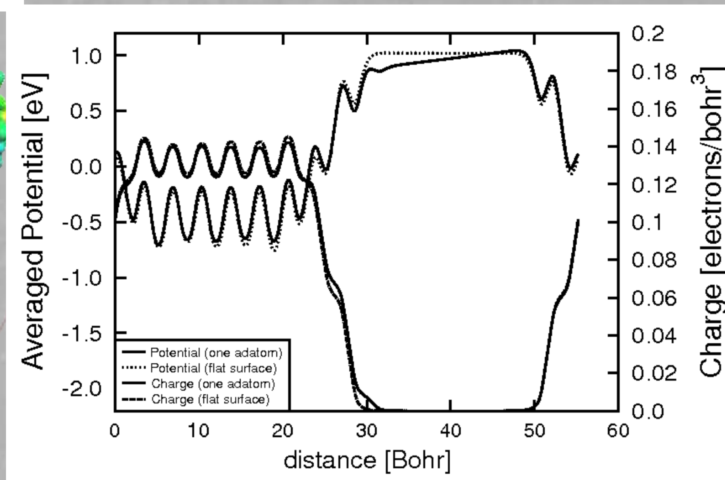


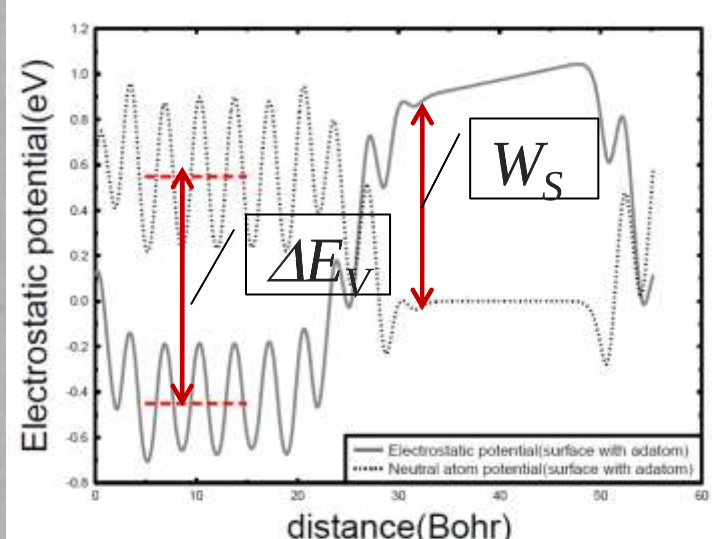
- DFT details:
  - Code: SIESTA
  - For exchange and correlations functionals the Perdew, Burke and Ernzerhof scheme of Generalized gradient approximation (GGA)
  - Slab organized in 8 layers+ 8 layers of vacuum
  - External field is added to calculate the electrostatic potential in the vacuum

	Single adatom		Two adatoms	
	DFT	ED-MD	DFT	ED-MD
Partial Charge, q_e	-0.032	-0.0215	-0.025	-0.0177

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

Workfunction near an adatom in Cu

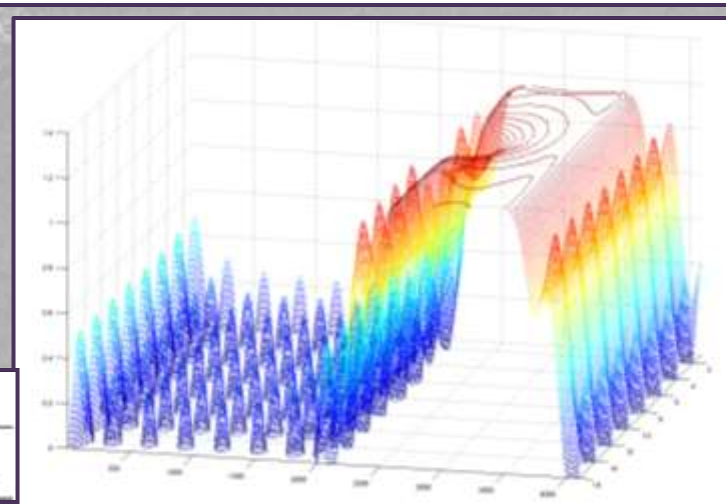




- We have calculated the workfunction for Cu surface when a single adatom is present

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

	Cu(100)	Cu(110)	Cu(111)
Φ LDA [27]	4.898	4.708	5.170
Φ(exp) [15]	4.599	4.490	4.980
Φ GGA (our calc.)	4.612	4.291	5.185

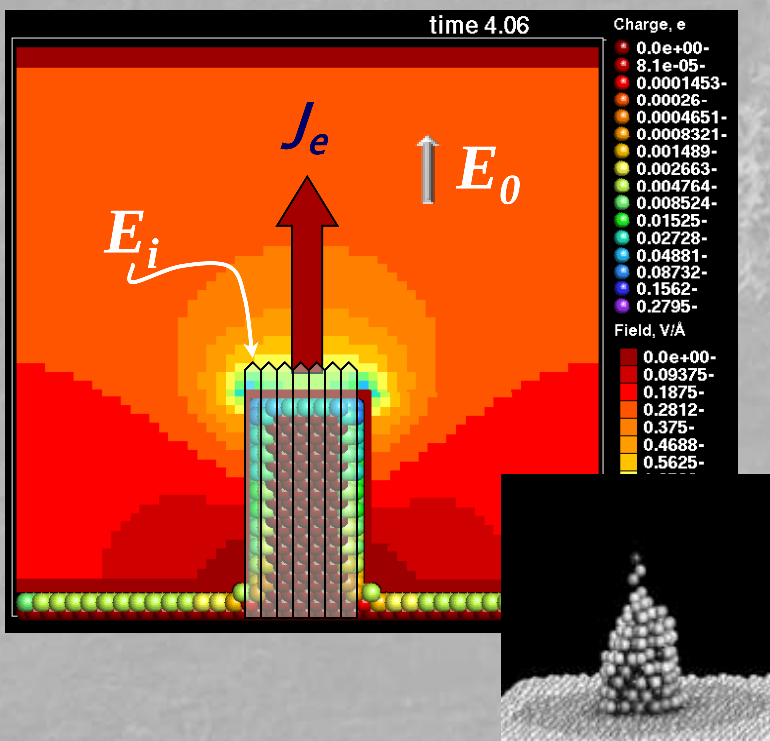


	Cu(100)	Cu(110)	Cu(111)
ΔΦ(adatom on small surface)	0.427	0.121	0.414

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.

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



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

Fowler-Nordheim constants:

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

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

The heat conduction from the tip has been implemented into MD

The heat conduction from the tip has been implemented into PARCAS by solving the heat conduction equation

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

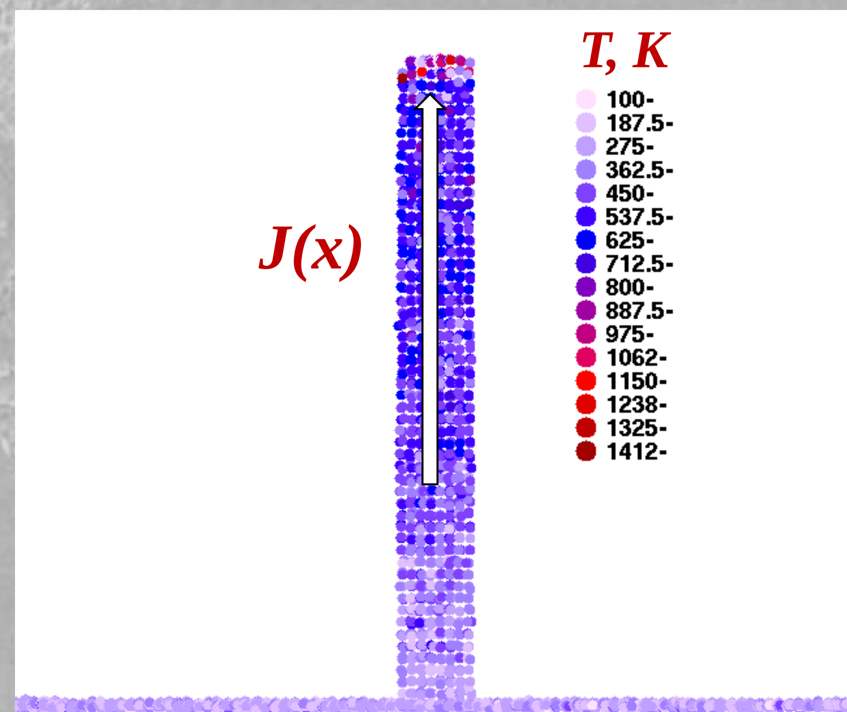
Here C_V volumetric heat capacity. *Phonons are implicitly present in classical MD*. In the equation we include only electron thermal conductivity given by the Wiedemann-Franz law

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

Where Lorenz number is found as

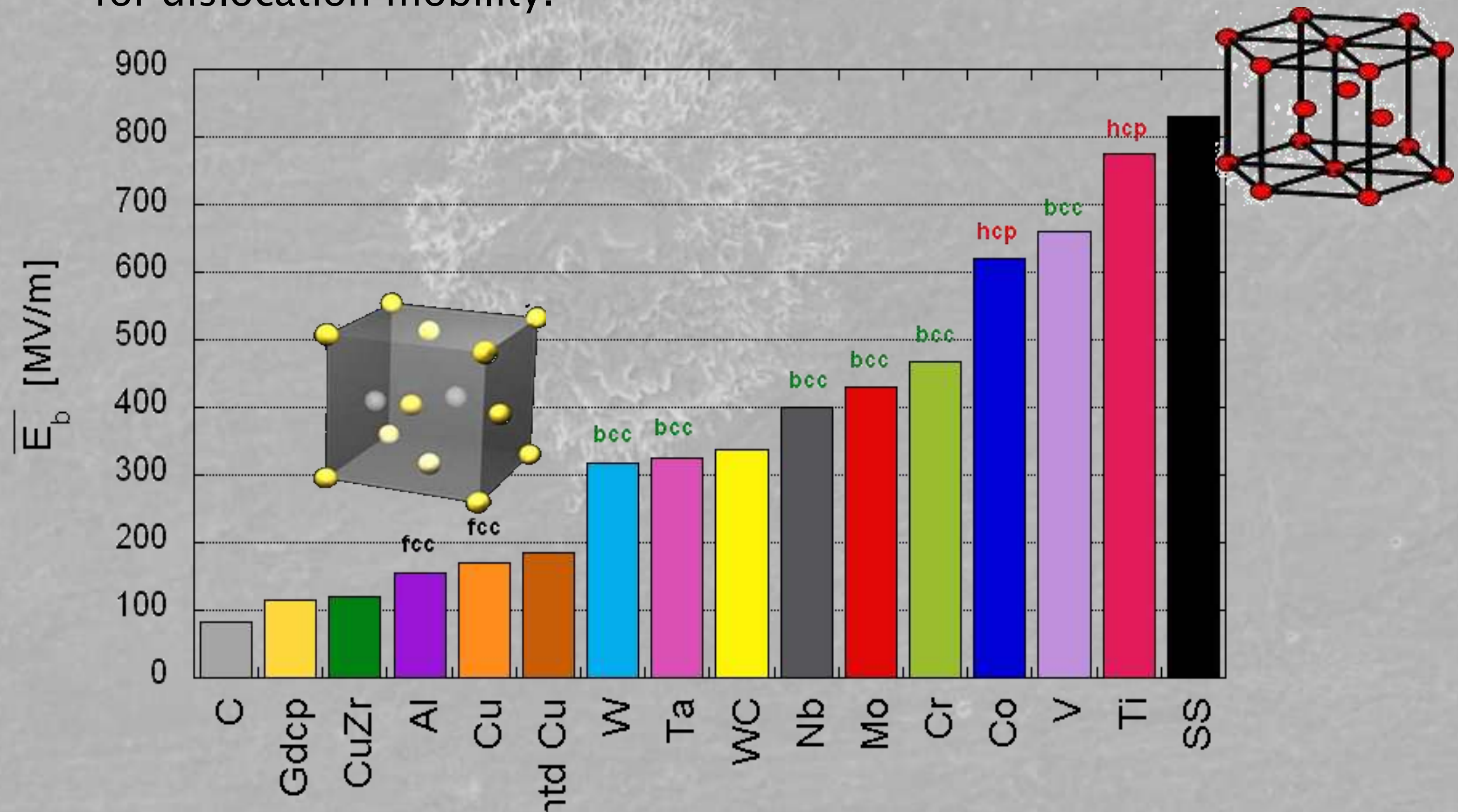
$$L = (\pi^2/3)(k_B^2) = 2.443\times10^{-8}\ \mathrm{W\Omega K^{-2}}$$

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

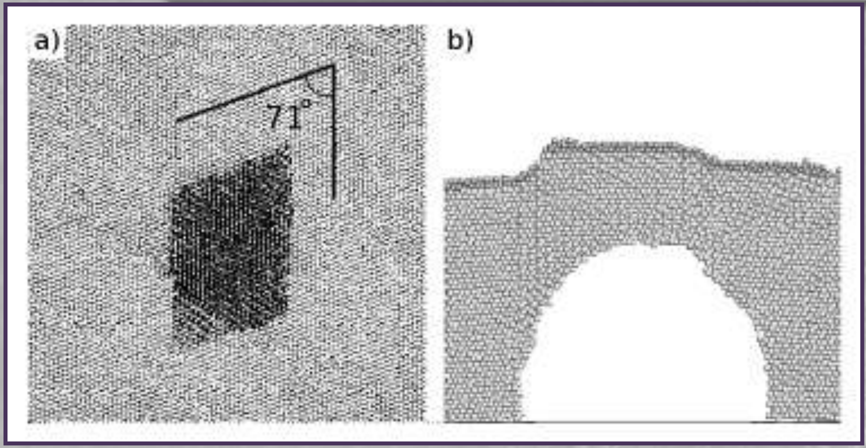


Recent experiment at CERN (CLIC)

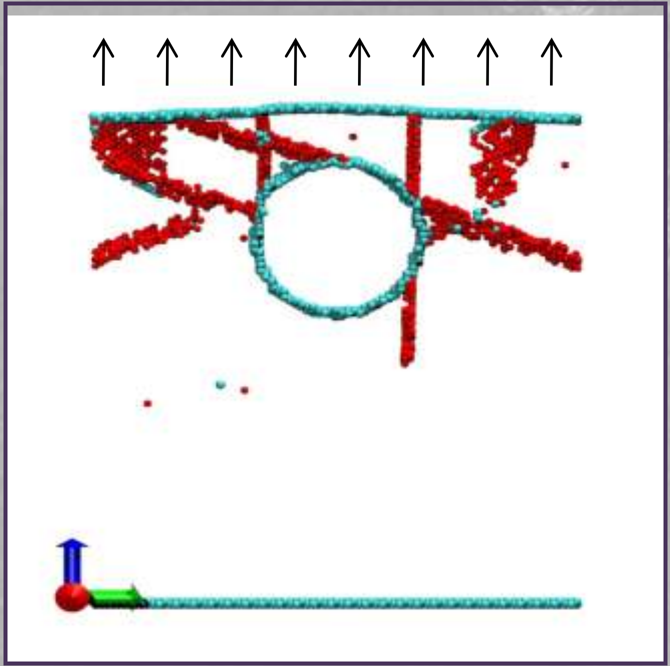
- The dislocation motion is strongly bound to the atomic structure of metals. In FCC (face-centered cubic) the dislocation are the most mobile and HCP (hexagonal close-packed) are the hardest for dislocation mobility.

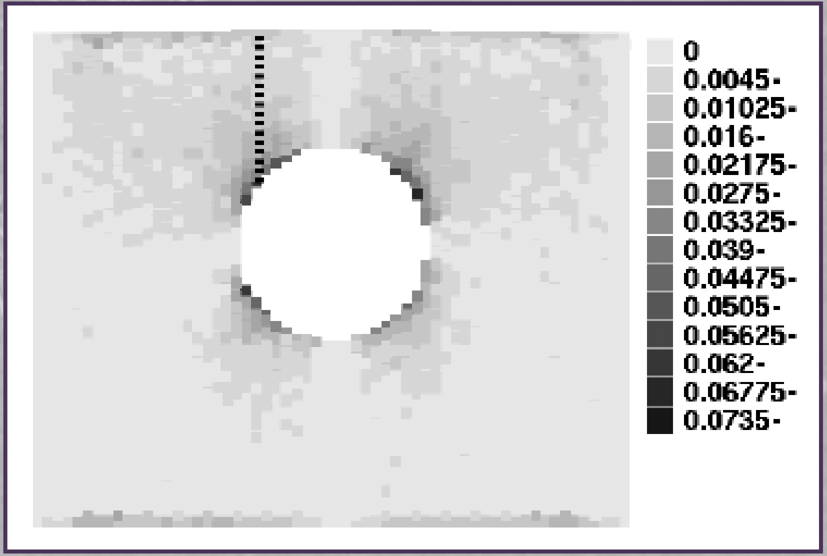


Void as a possible culprit?



- 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.

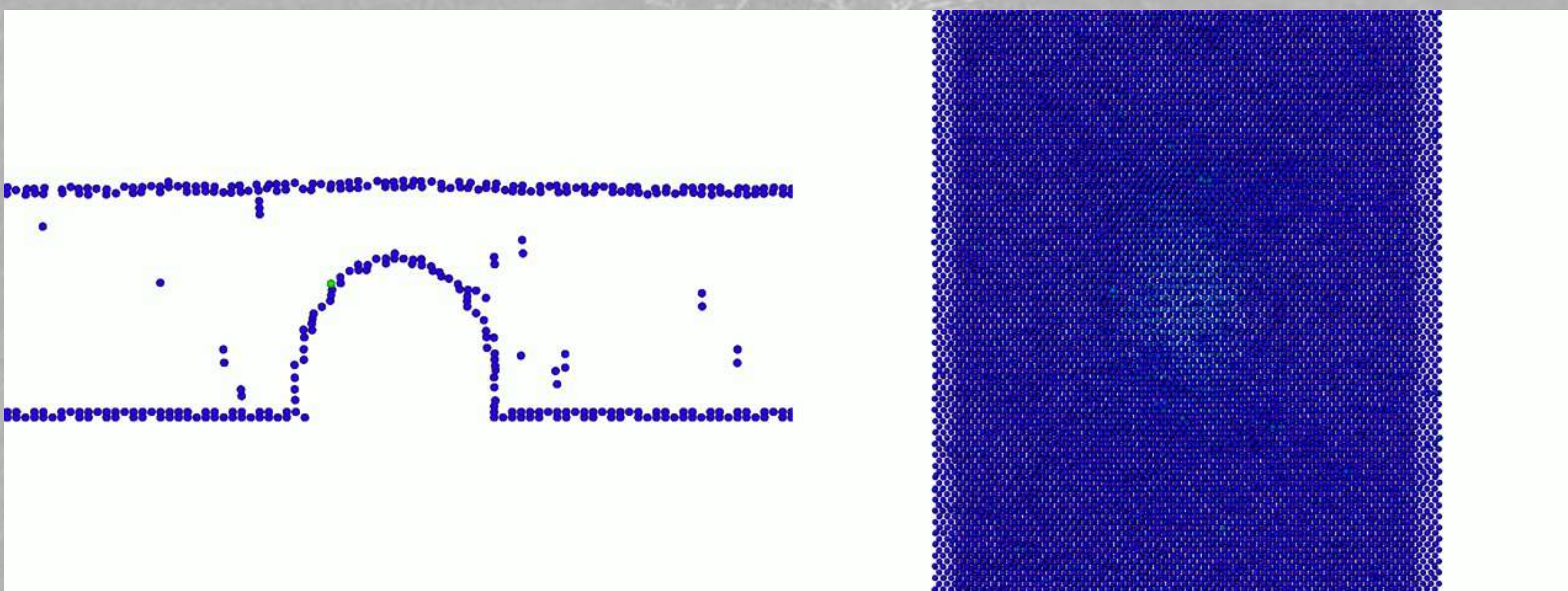




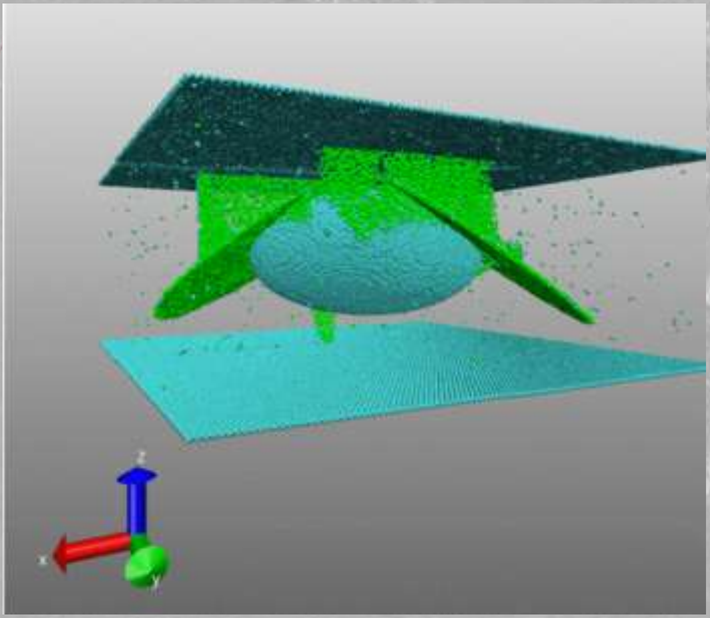
A. Pohjonen, F. Djurabekova, et al., Dislocation nucleation from near surface void under static tensile stress on surface in Cu, *Jour. Appl. Phys.* 110, 023509 (2011).

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

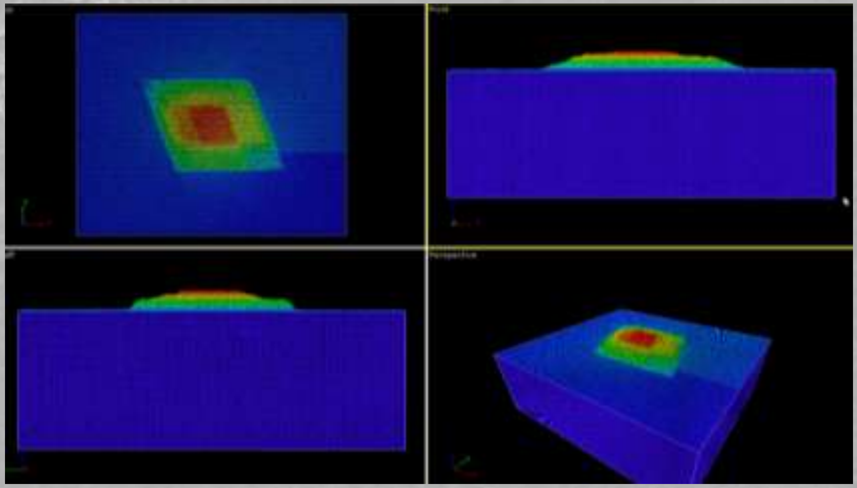
- Half–void of diameter 4nm in {110} Cu surface. (N of atoms≈ 170000 atoms…)
- E0=22 GV/m (exaggeration is required to simulate the dislocation within the MD time span)
- T = 600 K



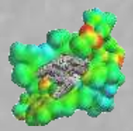
Dislocation reactions on a near surface void

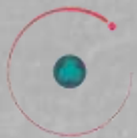


- A screw dislocation placed so that it intersects the void on a side, showed a cross-slip behavior leading to the atom step on the surface. This mechanism eventually combines with the previous mechanism, but to ignite this process less stress is required (in our simulations 1.7 GPa against 3 GPa).



From tips to plasma:
From FE to discharge currents



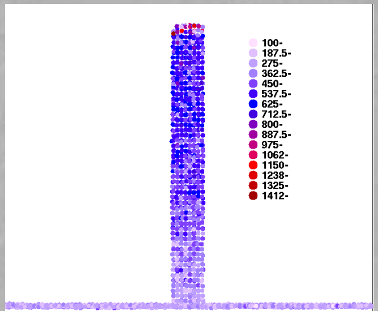


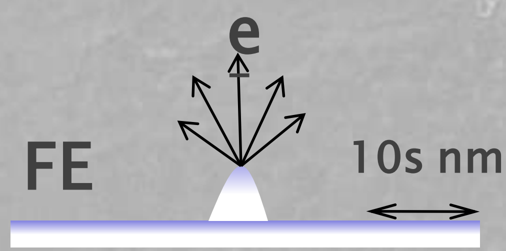
- In real life we can observe the full dynamic range of a vacuum discharge:
  - > 10s pA in ‘weak’ FE phase
  - Space charge limited ‘strong’ FE phase, typically ~ nA – μA
  - Discharge current, up to 10 – 100 A

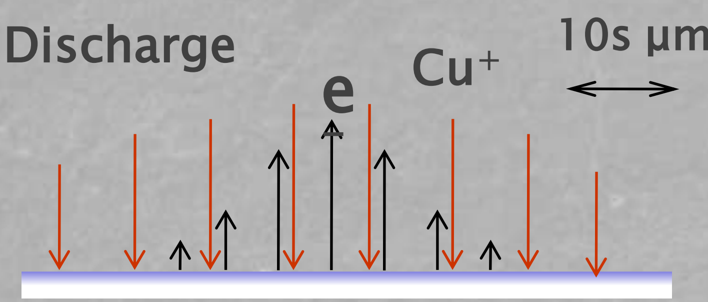
Up to 12 orders of magnitude difference

- 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

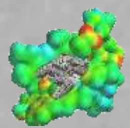


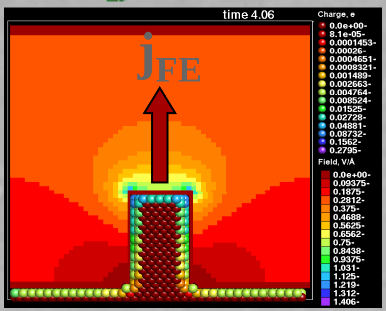


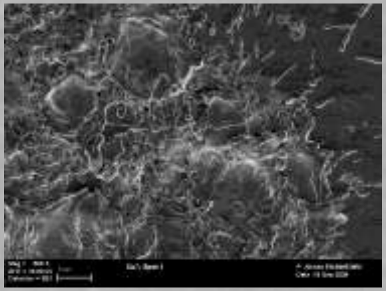


Plasma evolution

Corresponding to experiment...



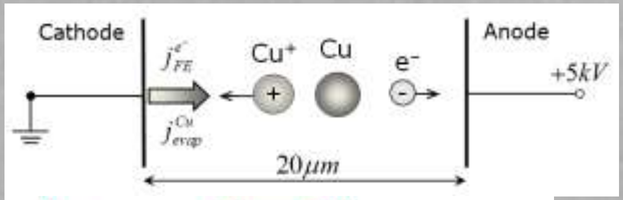


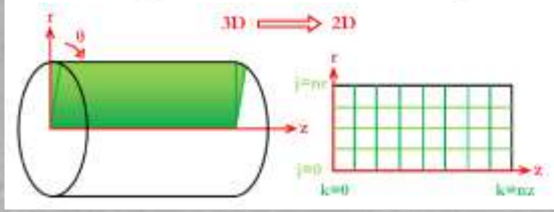


Up to now we have electrostatic PIC-MCC codes:

1d3v

the 2D-model

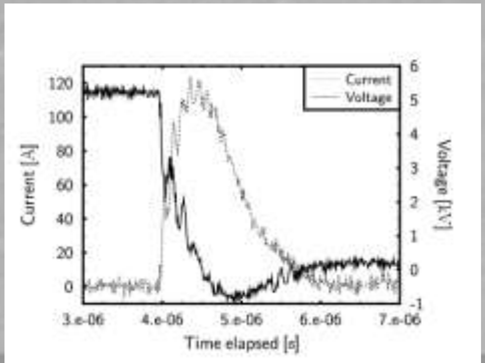




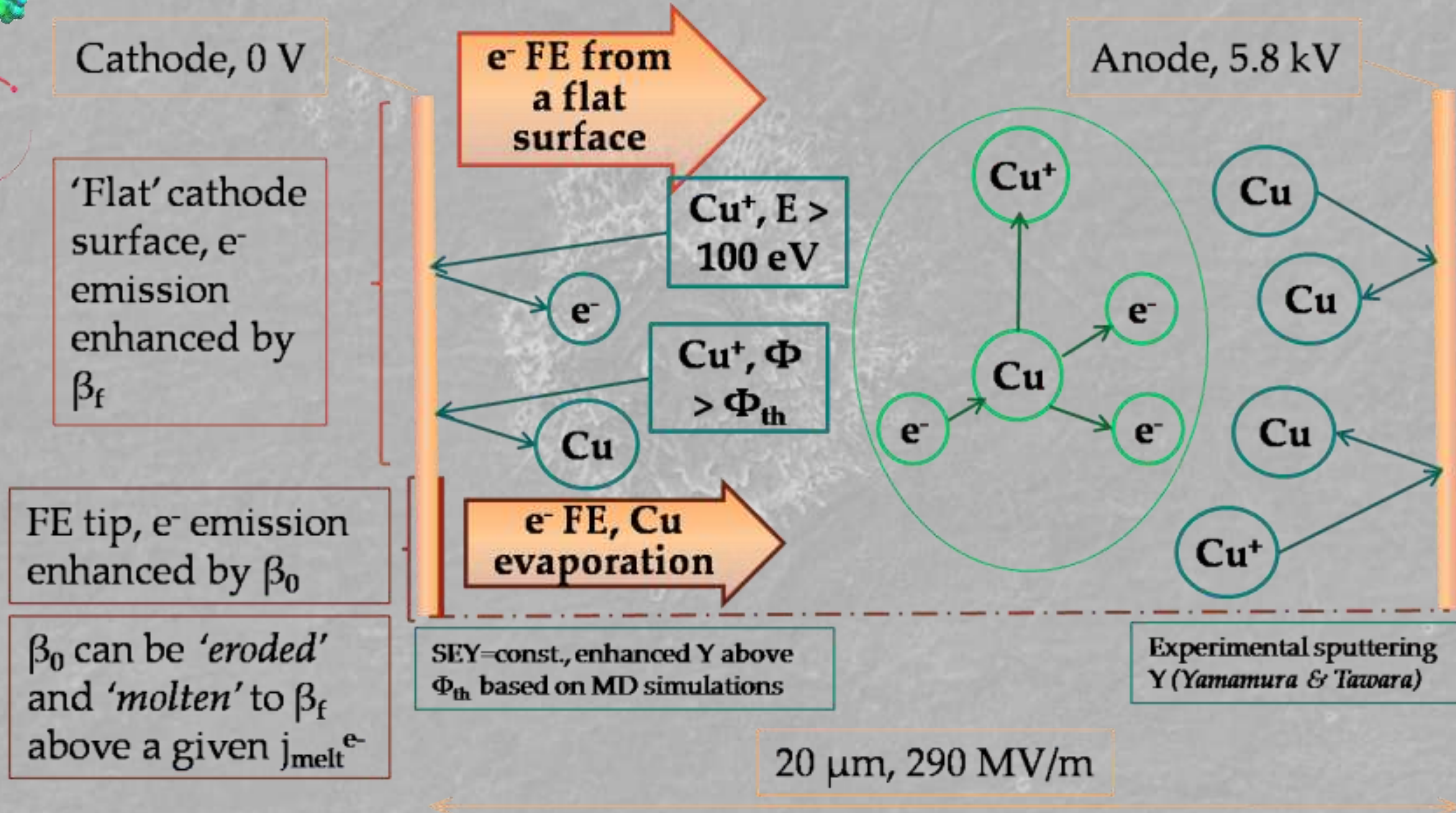
Provide us with a link between

1. Micro- & macroscopic surface processes: Triggering (nano-scale) → plasma → crater formation (visible effect)
2. Theory & experiments: Using reasonable physical assumptions (theory), the aim is to predict the evolution of measurable quantities (experiment)

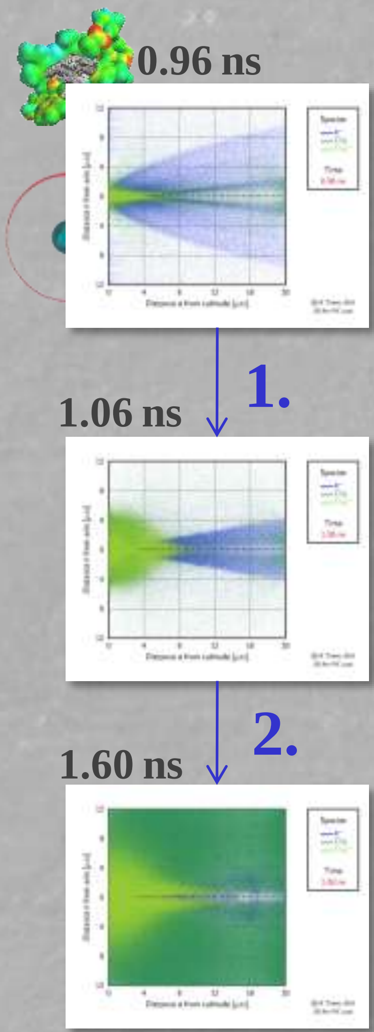
H. Timko, K. Matyash, R. Schneider, F. Djurabekova, K. Nordlund, A. Hansen, A. Descoeudres, J. Kovermann, A. Grudiev, W. Wuensch, S. Calatroni, and M. Taborelli , *Contrib. Plasma Phys. 5*1, 5-21 (2011)



Processes included in plasma simulations



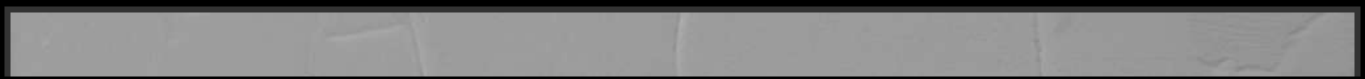
Observations

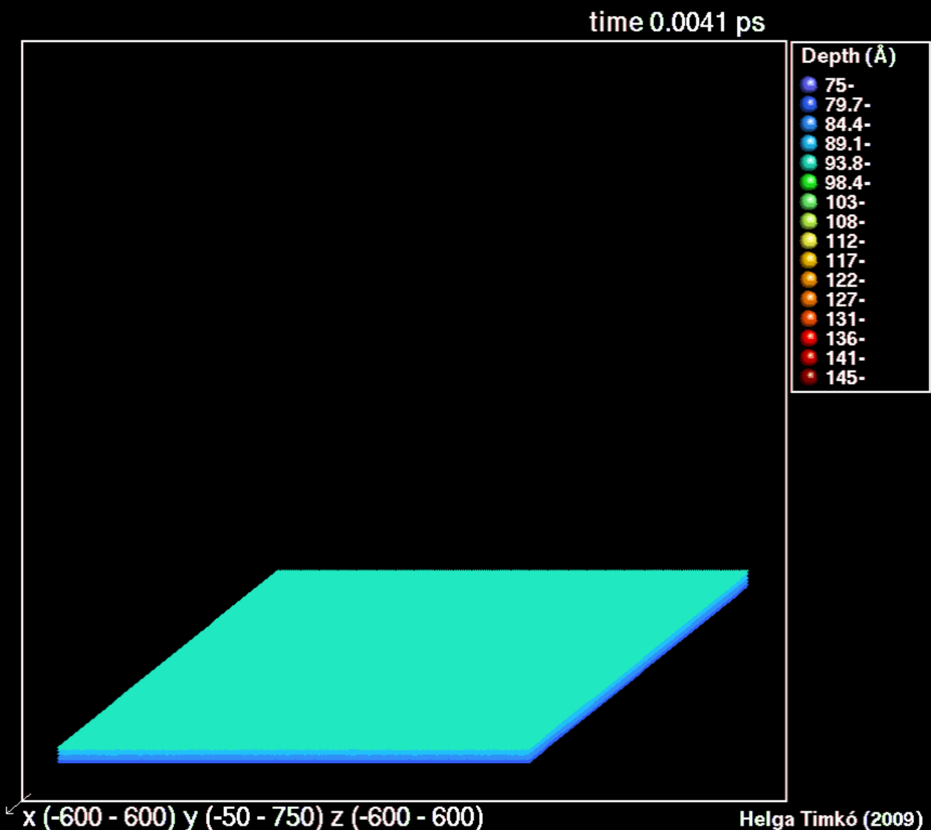


- Fully cathode dominated phenomenon
- Although FE starts from a small area, the discharge plasma can involve a macroscopic area on the cathode
- Transitions seen:
  1. Transition from strong FE to a small discharge plasma
     - Sudden ionisation avalanche
     - A plasma sheath forms, the plasma becomes 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

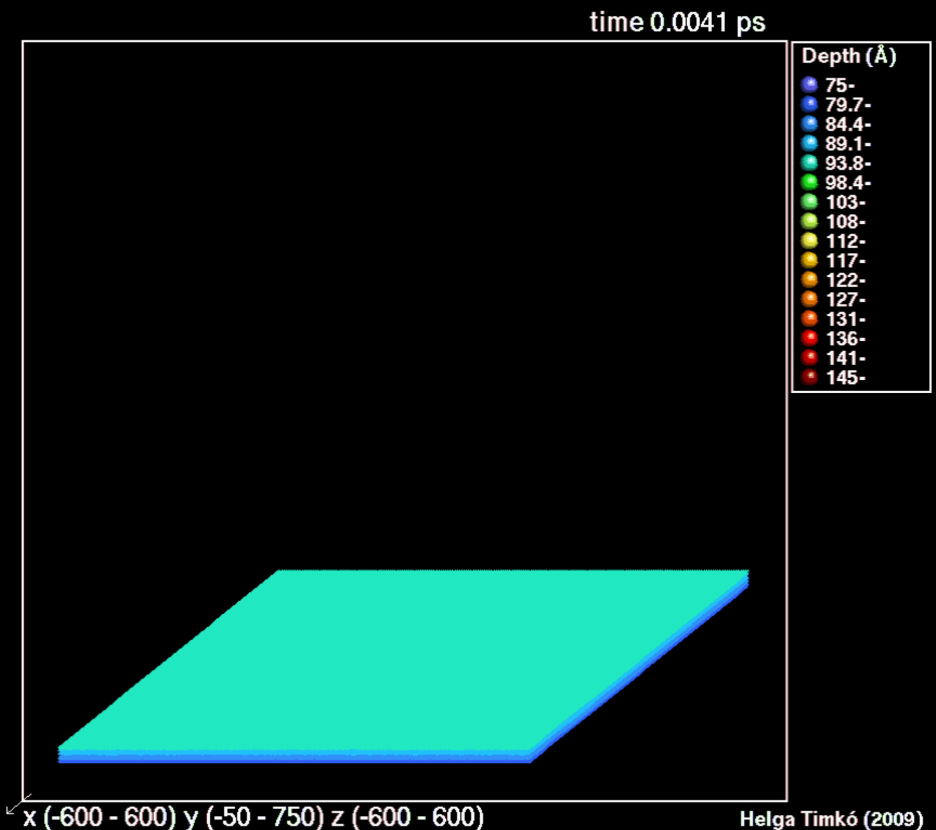
Huge fluxes of accelerated ions are the reason for surface damage

Ion fluxes leave rims of peculiar shape



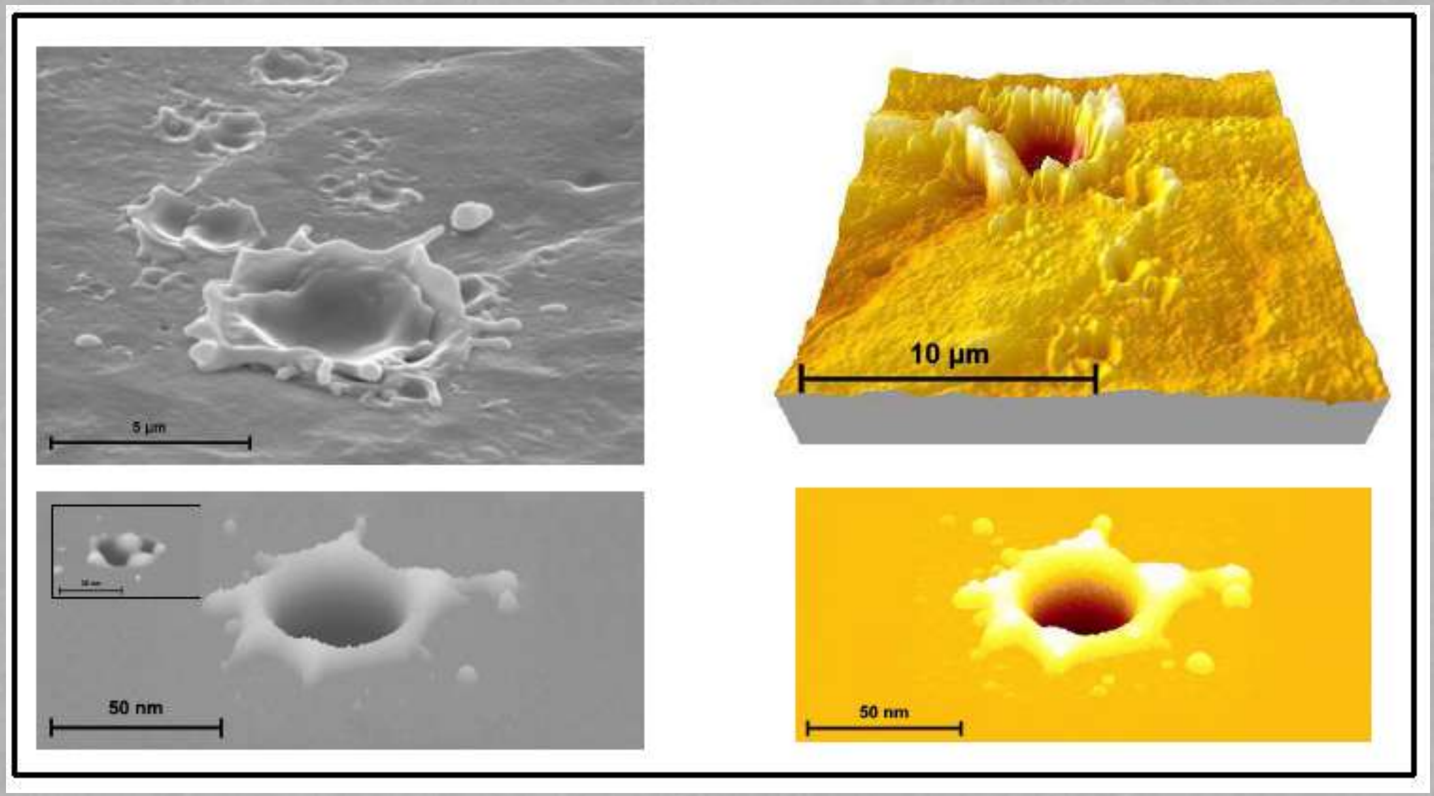


Damage caused by thermal heating in Cu, 100 ions, on r = 15 nm spot



DC arc plasma damage in Cu, 100 ions, on r = 15 nm spot

AFM measurements of single spark event, produced at CERN

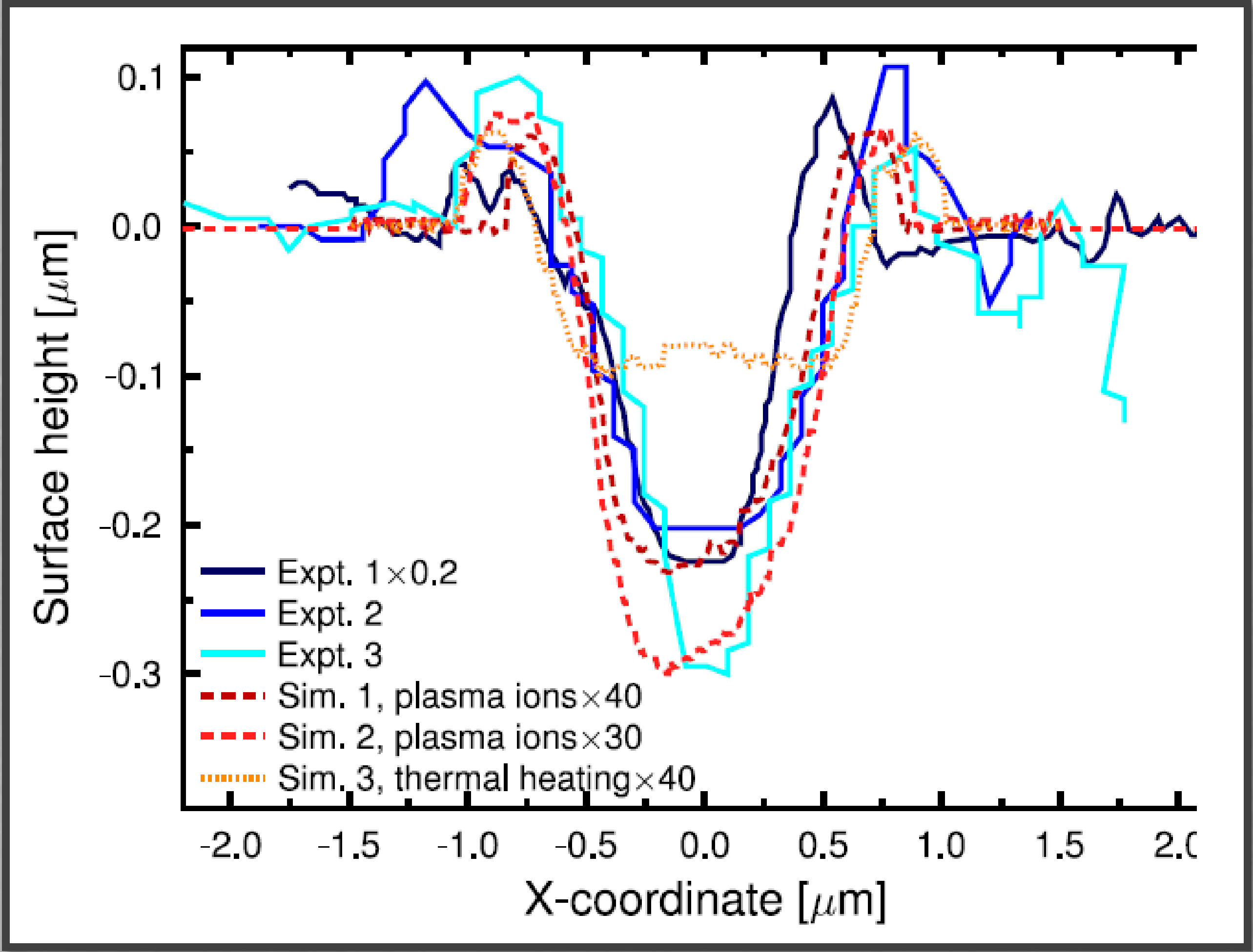


Top left: tilted SEM image (CERN)

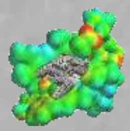
Top right: tilted AFM (atomic force microscopy)

Below: simulation images coloured with respect to the height of surface topography

Crater shape profiles from experiment and simulation



H. Timko, F. Djurabekova, *et al.* *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 started in parallel. We start, continue and develop intense activities to cover all possible aspects.
- Most recently our modeling has shown:
  - The trigger of the sparks is explained by plasma discharge;
  - Plasma is fed from the tips grown under the high electric field
  - Tip growth can be explained by the natural relaxation of stresses inside of material by the dislocation motion

- Fundamental physics
- Beam proc.
- Sputtering
- Oxides ceramics
- Ionic crystals
- Glass
- High Tc oxides
- Polymers
- Nuclear materials
- Applications
- Nanostructures

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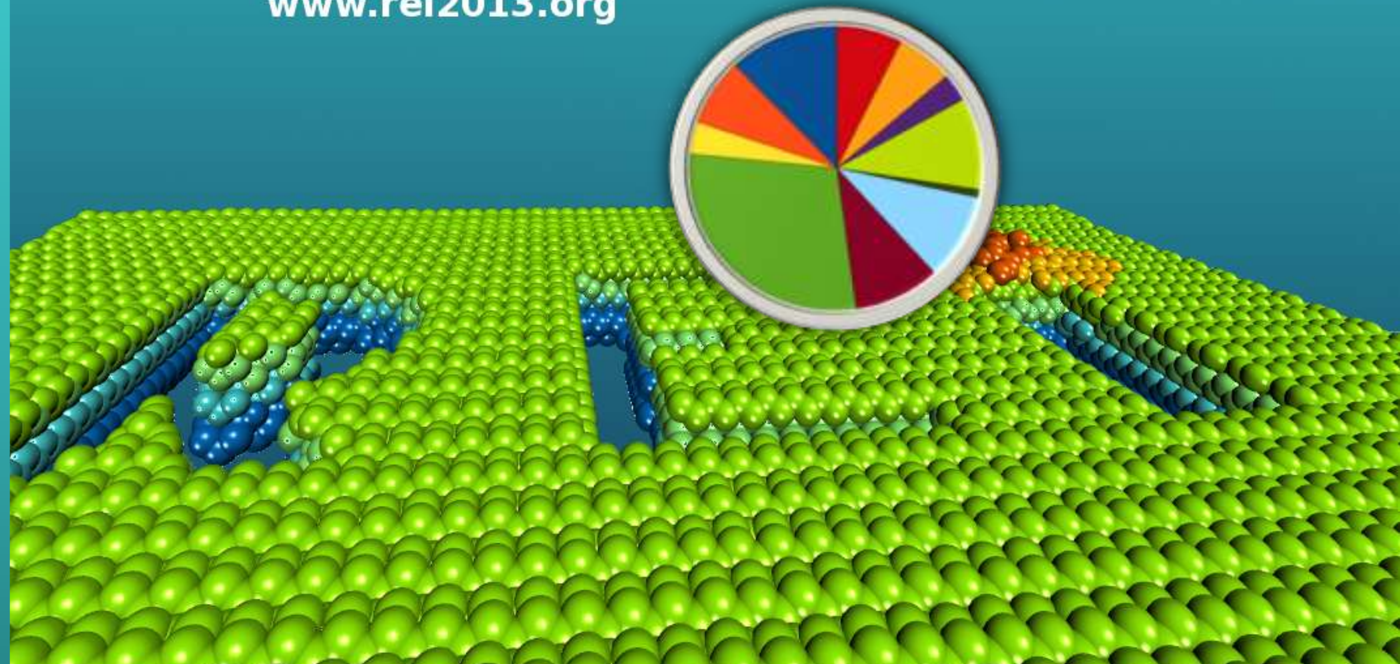

WELCOME!

Thank you!