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HIP

Multiscale modelling of electrical breakdown at high electric field

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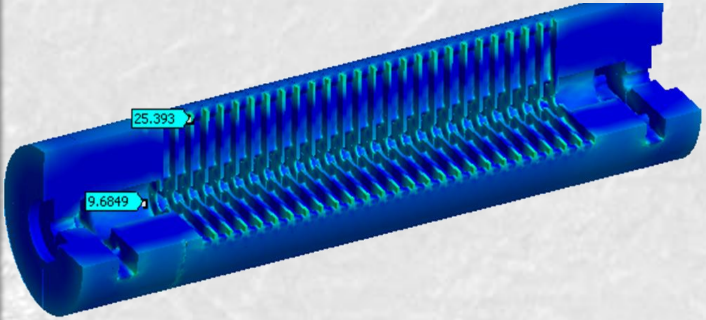
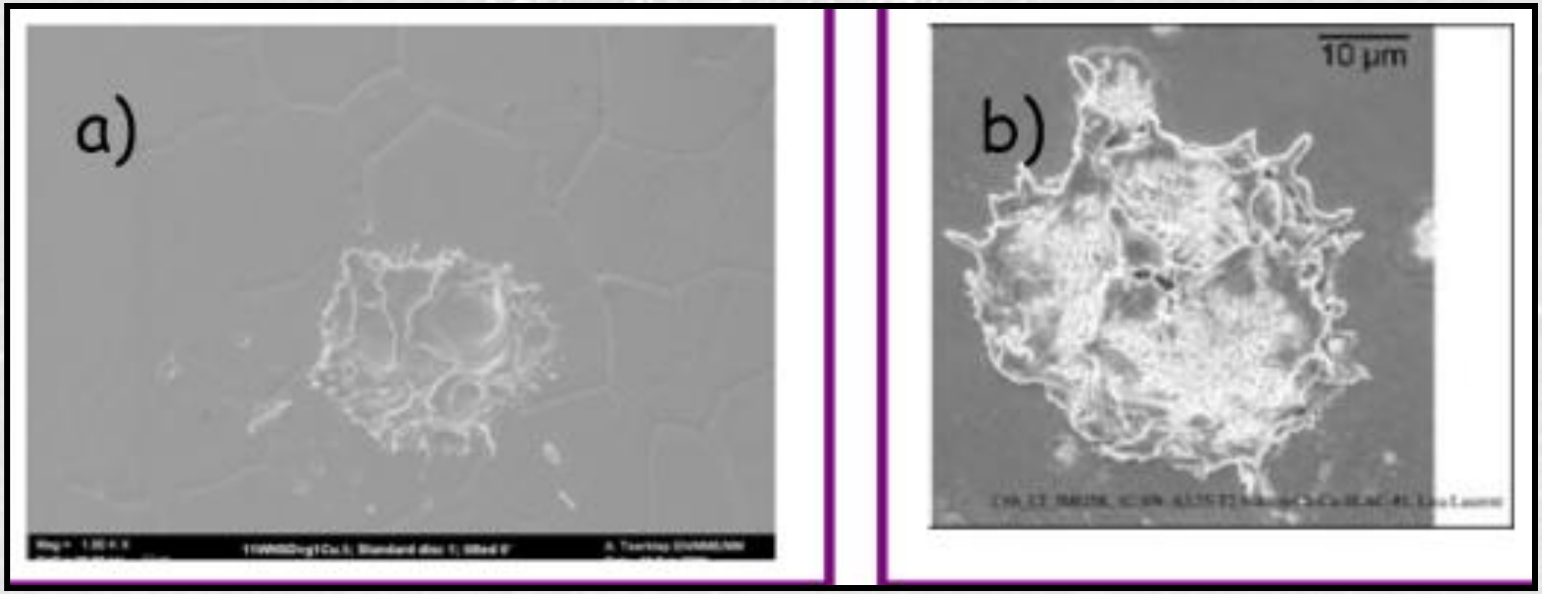
Outline

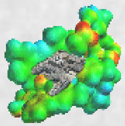
- Tools in use
- Electrical breakdown:
  - Multiscale Model
    - Effect of high electric fields on metal surface
    - Plasma+surface damage
- Physically motivated fitting law for breakdown dependence on E
  - Dislocations major “convicts” for the breakdown initiation?
- Summary

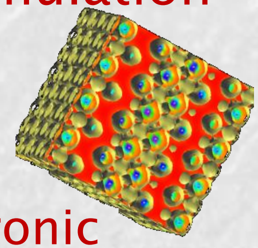
DC *vs* RF



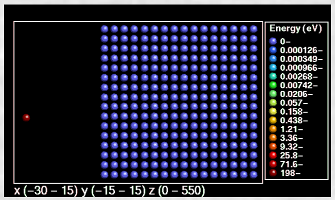


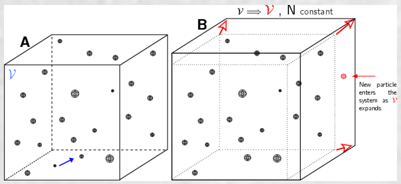
Tools in use:

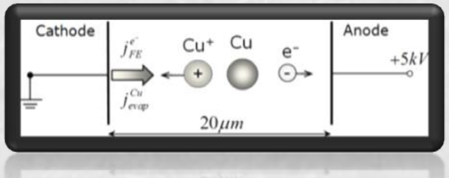




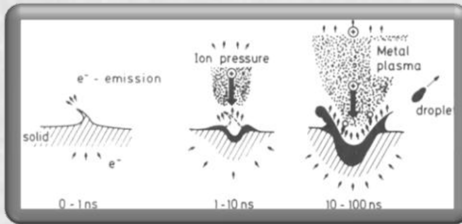
- In our group we use all main atomic-level simulation methods:
  - Density functional theory (DFT)
    - Solving Schrödinger equation to get electronic structure of atomic system
  - Molecular dynamics (MD)
    - Simulation of atom motion, classically and by DFT
  - Kinetic Monte Carlo (KMC)
    - Simulation 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!

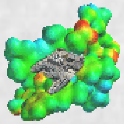






Multiscale model to simulate electrical breakdown)





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)

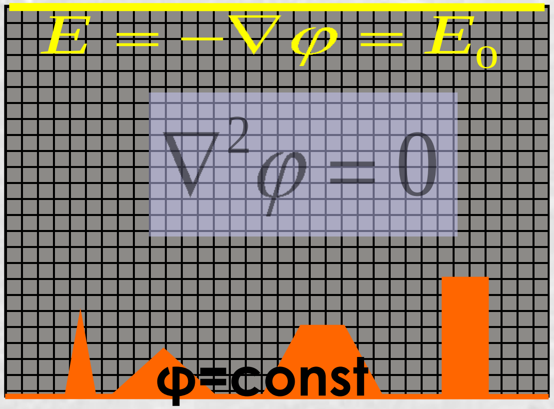
~10s ns

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

~

Some details: Stage 2

- Atoms move according Molecular dynamics algorithm, solving Newton equations of motion $\ddot{\vec{r}} = \frac{\vec{F}}{m_{at}}; \vec{F} = -\nabla V(\vec{r}_i)$
- But in ED&MD hybrid code $\vec{F} = -\nabla V(\vec{r}_i) + \vec{F}_L + \vec{F}_C$ for surface atoms as due to the excess or depletion of electron density (atomic charge)
- Gauss law given by the 'pillbox' technique a surface charge per area $\sigma = \varepsilon_0 \mathrm{E}$ is applied to calculate the charges; E is a field given by solution of Laplace equation with the mixed boundary condition



(conductive material)

F. Djurabekova, S. Parviainen, A. Pohjonen and K. Nordlund: "*Atomistic modelling of metal surfaces under electric fields: direct coupling of electric fields to a molecular dynamics algorithm*", PRE 83, 026704 (2011)

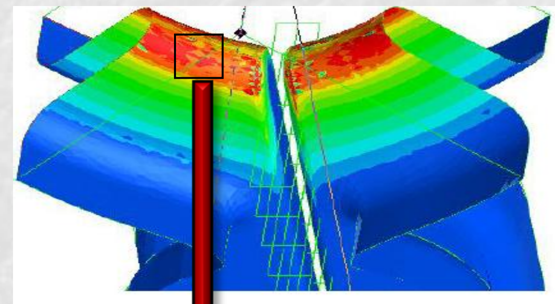
External electric field: classical electrodynamic approach

Gauss law states

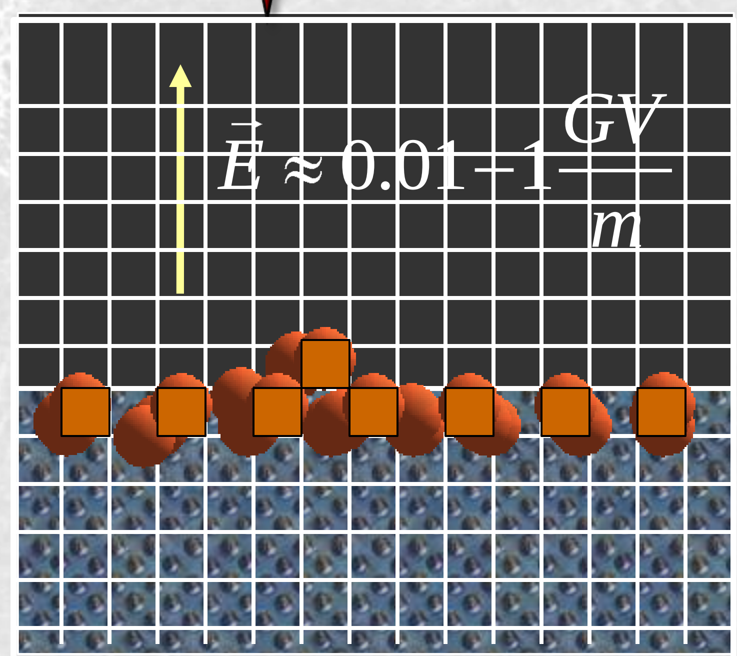
$$\sigma = \frac{Q_{surface}}{A_{surface}} = \varepsilon_0 E$$

Due to the external electric field the surface attains charge

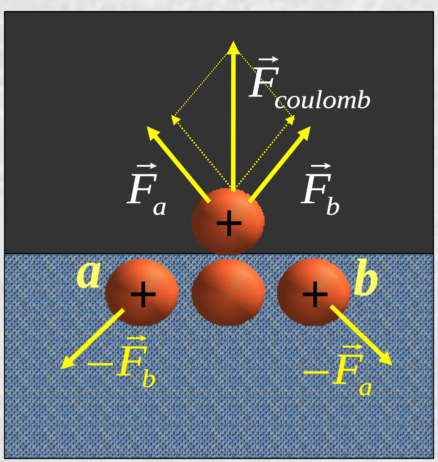
Macroscopic field to…



…the atomic level:



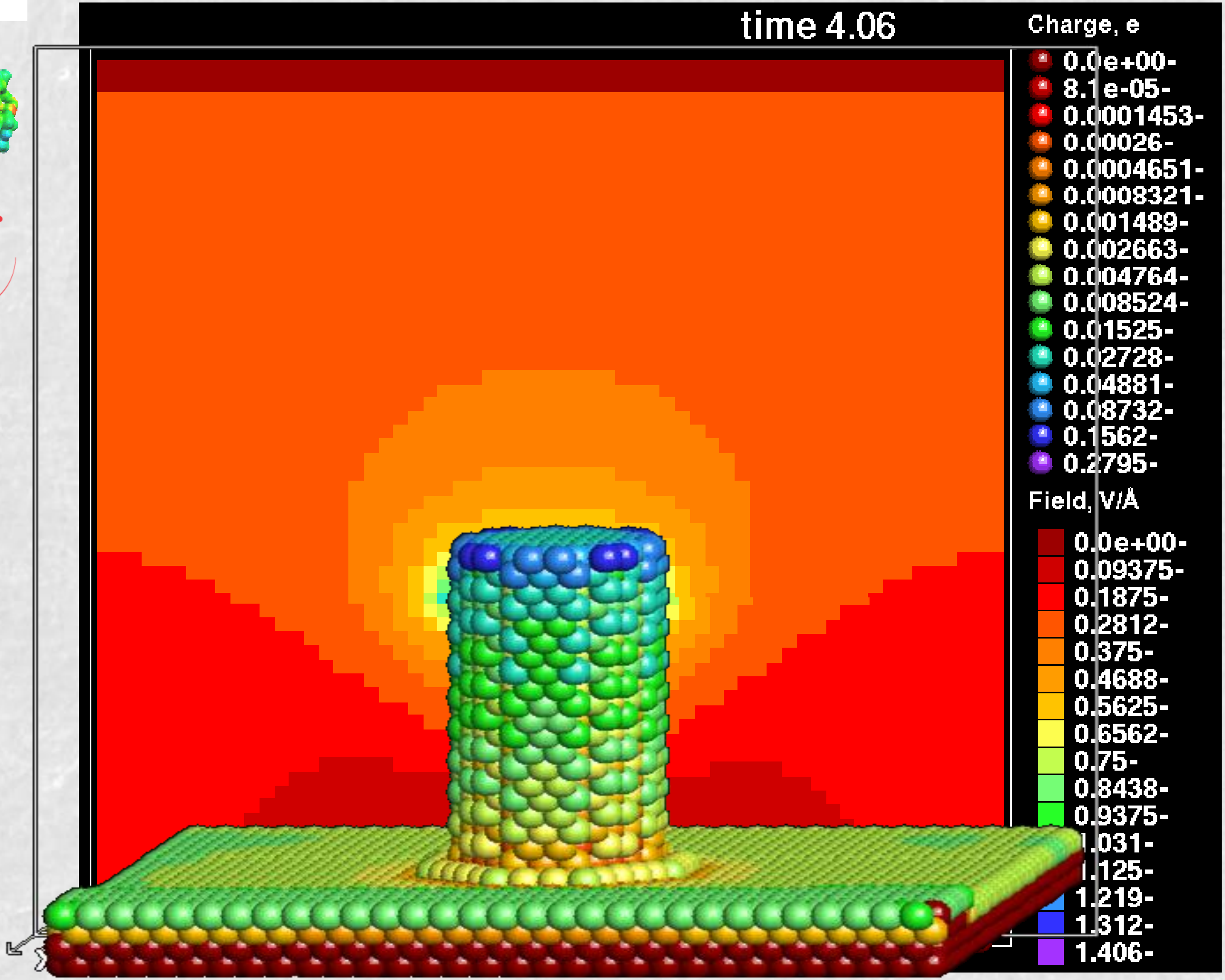
Two electric forces modify the motion of charged atoms:



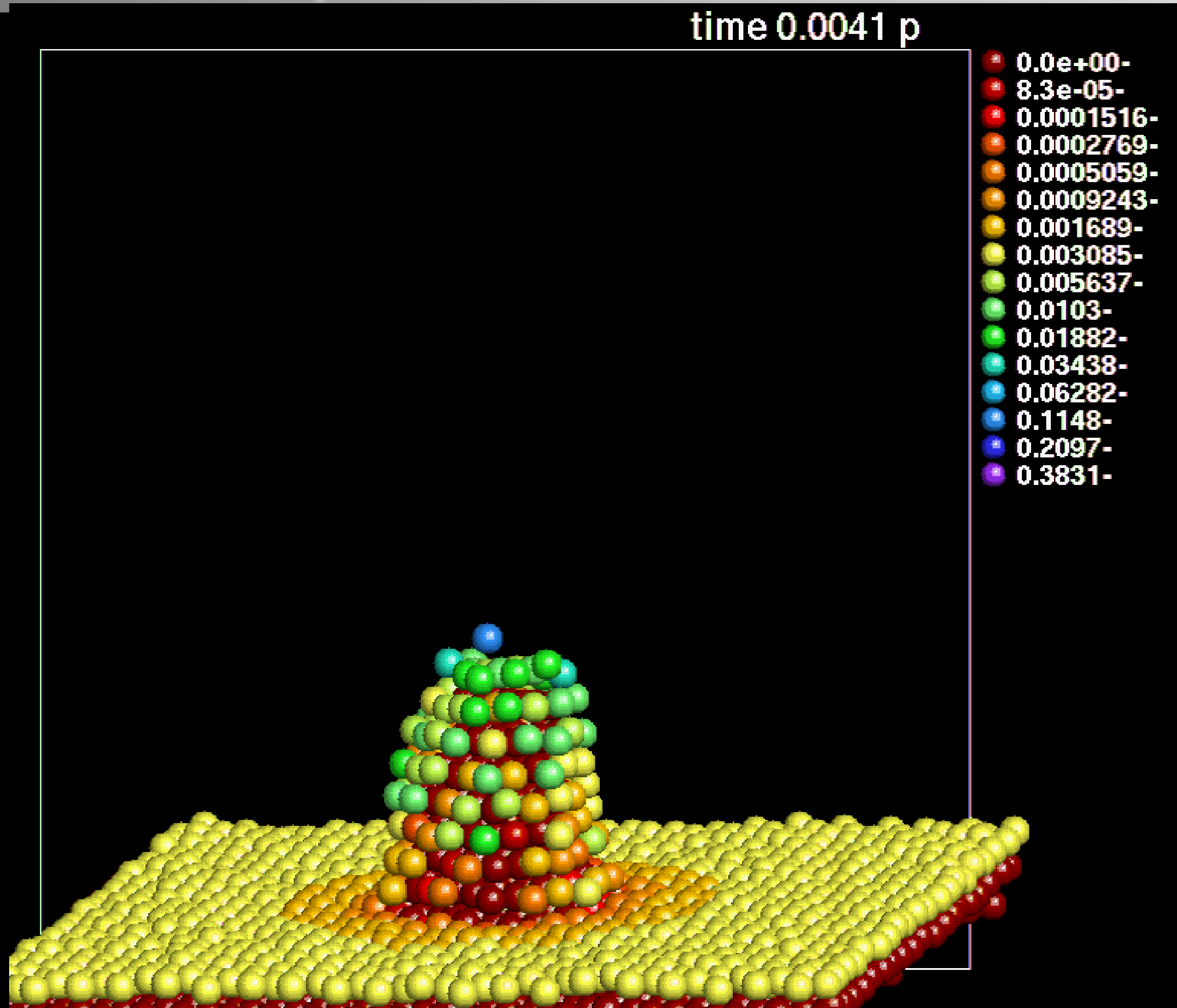
$$\vec{F}_L = \vec{E}q$$

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

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

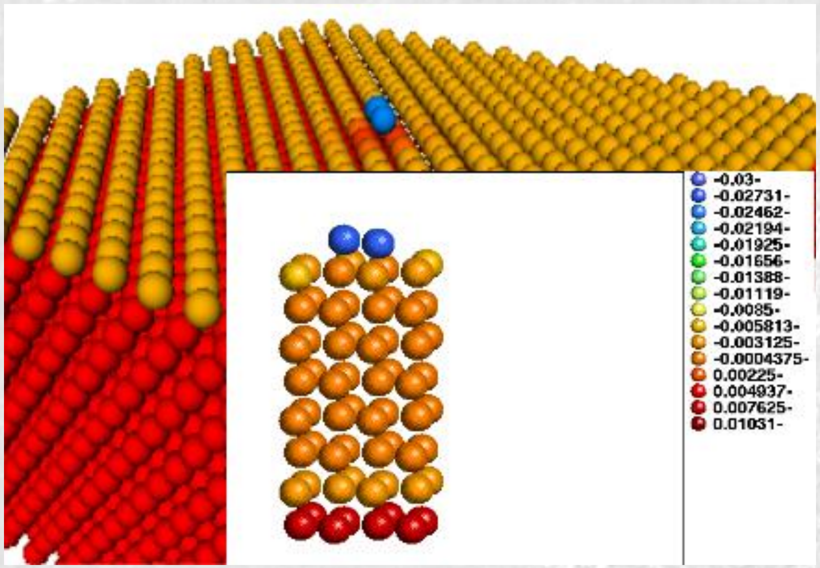


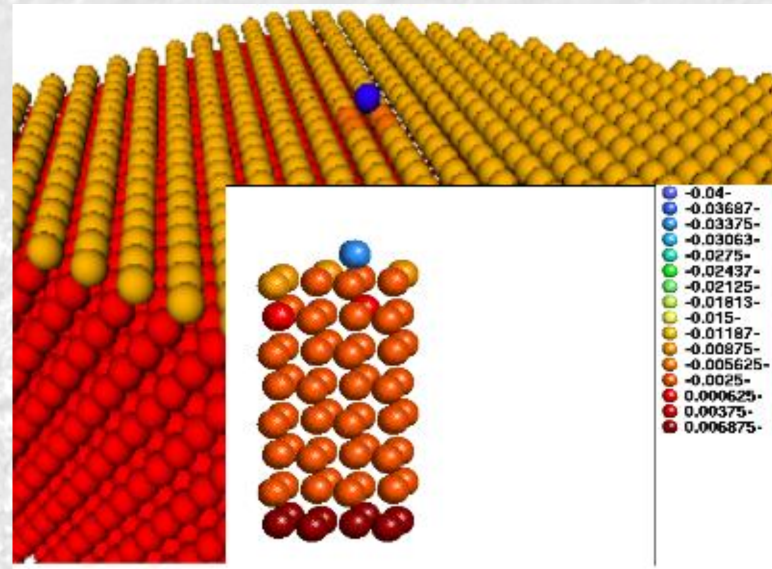
Atom/cluster evaporation from Cu(100) @ 500 K, E_0 ~ 1 GV/m



Aarne Pohjonen

Results of the recent work

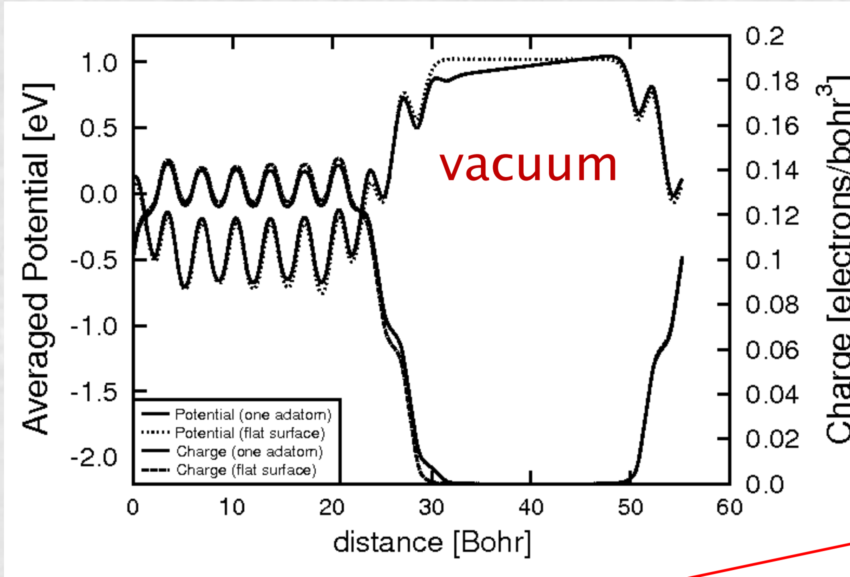




	Single adatom		Two adatoms	
	DFT	ED-MD	DFT	ED-MD
Partial Charge, q_e	-0.032	-0.0215	-0.025	-0.0177

	Flat surface		Surface with one adatom
	present DFT	experiment [16]	
Work function, eV	4.61	4.46 ± 0.03	4.30

Calculation of work function

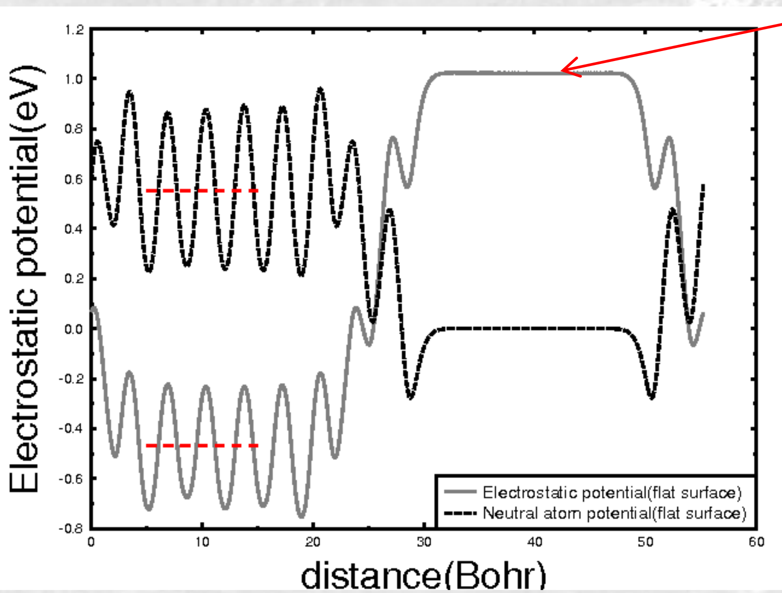


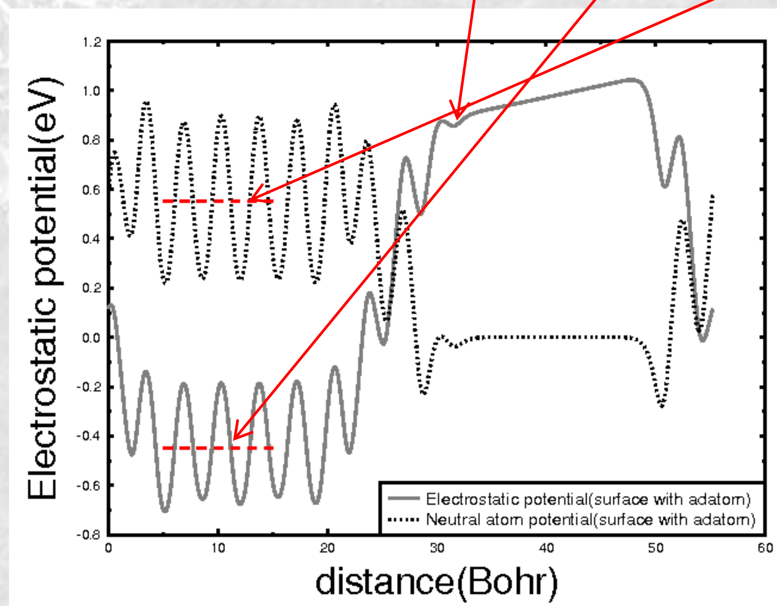
Distribution of electrostatic potential and electronic density as a function of distance from the bottom of the cell

$$W = \Delta E_v + \Delta V$$

$$\Delta E_v = E_{vacuum} - E_{Fermi}$$

$$\Delta V = \langle \delta V^H \rangle = \langle V^H_{i+e} \rangle - \langle V^{NA} \rangle.$$





Field emission current induces a temperature gradient in the surface protrusion

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

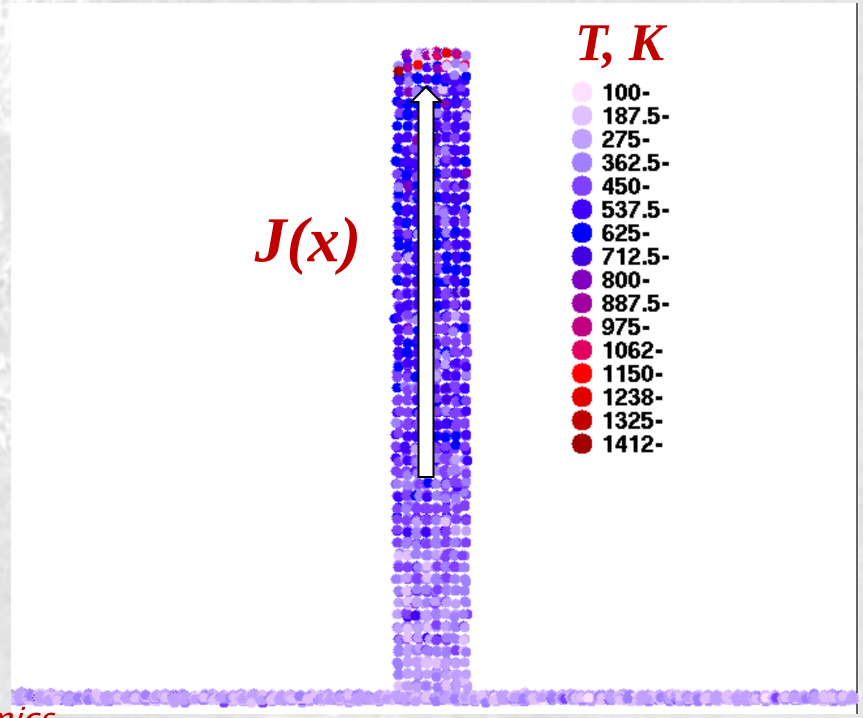
$$\frac{\partial T(x,t)}{\partial t} = \frac{1}{C_V}\left(\rho\ T(x,t)\ J(x)^2 + k_e(T)\frac{\partial^2 T(x,t)}{\partial x^2}\right)$$

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

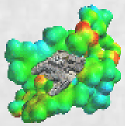
$$K_e(T) = \frac{LT}{\rho(T)}$$

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, *Implementation of electronic processes into molecular dynamics simulations of nanoscale metal tips under electric fields*, Comput. Mater. Sci. 50, 2075 (2011).



PIC : phenomena taken into account to simulate plasma – Three species: e^-, Cu, Cu^+

Initial Cu, e^-

- Cu evaporation, enhanced electron field emission from a field emitter tip (Fowler-Nordheim eq)

$$j_{FE} = a_{FN} \frac{eE_{LOC}}{\phi t(y)^2}^{2} e^{-b_{FN}\frac{\phi^{3/2}v(y)^2}{eE_{loc}}}, \quad \text{where } E_{loc} = \beta \cdot E$$

$$t(y) = 1,\ v(y) = 0.956 - 1.062y^2 \quad \text{where } y = \sqrt{\frac{e^3 E_{LOC}}{4\pi\varepsilon_0 \phi^2}}$$

- Electron field emission also from the flat cathode surface

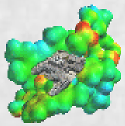
Create ions

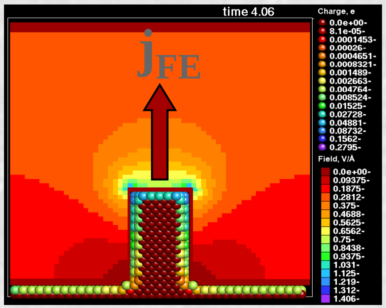
- Collisions, esp. ionisation collisions

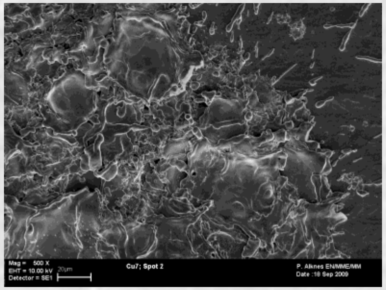
More e^- and Cu

- Sputtering of Cu neutrals at the walls, enhanced MD yield at the cathode above a certain ion flux
- Secondary electron yield due to ion bombardment **at the cathode**

Plasma evolution





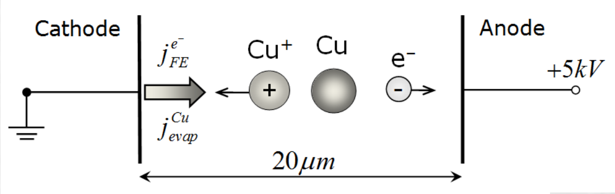


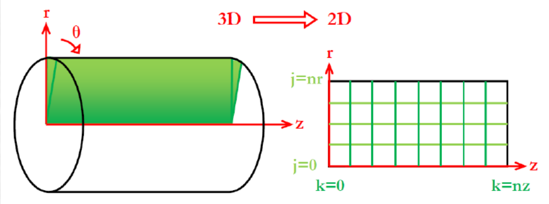
Up to now we have electrostatic PIC-MCC codes:

1d3v;

the new 2D-model

Corresponding to experiment...

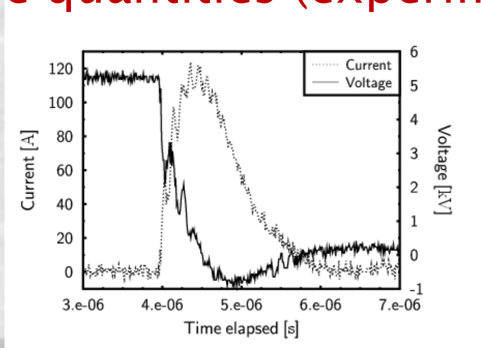


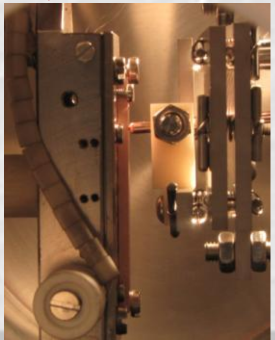


Provide us with a link between

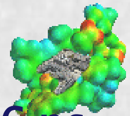
1. Micro- & macroscopic surface processes: Triggering (nano-scale) → plasma → crater formation (visible effect)
2. Theory & experiments: Using reasonable physical assumptions (theory), the aim is to predict the evolution of measurable quantities (experiment)

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 , "*A One-Dimensional Particle-in-Cell Model of Plasma Build-up in Vacuum Arcs*", Contrib. Plasma Phys. 51, 5-21 (2011)

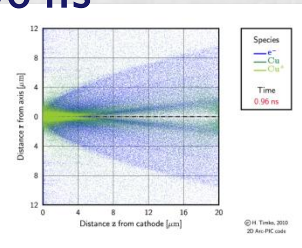




Observations

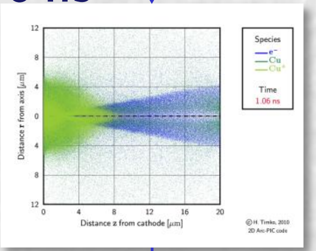


0.96 ns



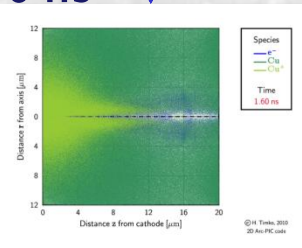
1.

1.06 ns



2.

1.60 ns

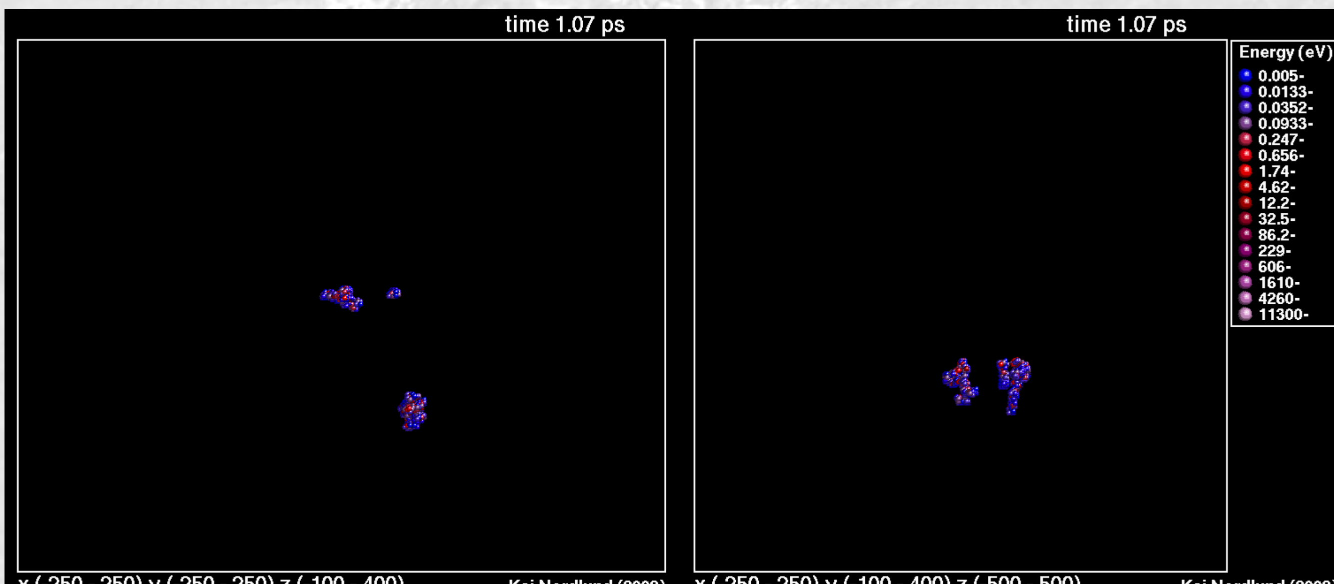


- Fully cathode dominated phenomenon
- Although FE starts from a small area, the discharge plasma can involve a macroscopic area on the cathode
- Transitions seen:
  1. Transition from strong FE to a small discharge plasma
     - Sudden ionisation avalanche
     - A plasma sheath forms, the plasma becomes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

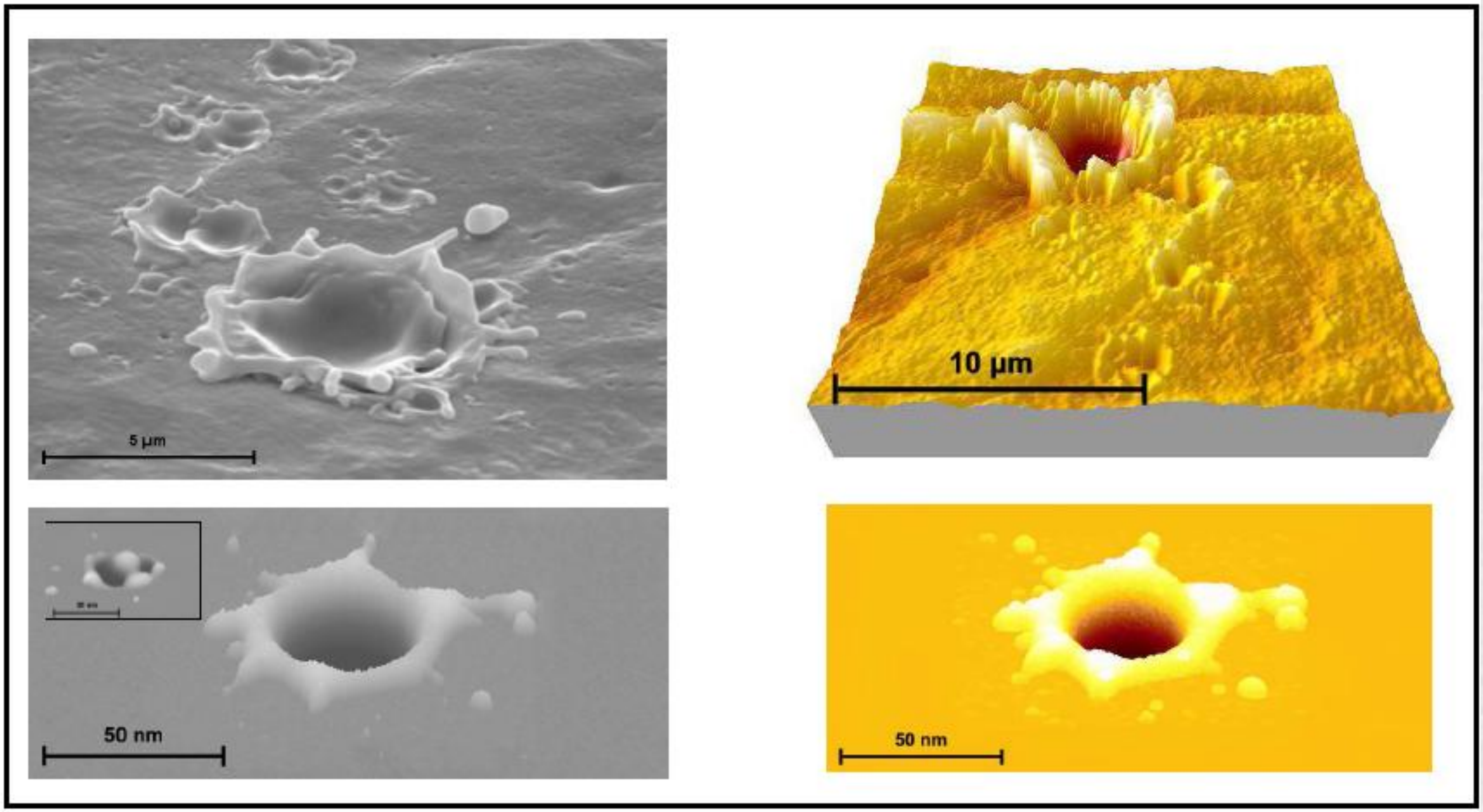
Classical MD simulations damage

- MD simulations of surface bombardment on a given area *A*
  - Ion flux and energy distribution corresponded *exactly* to that from the 1D PIC simulations!
    - Flux of ~10^{25} on eg. r=15 nm circle => one ion/20 fs!!

Top view **Side view**

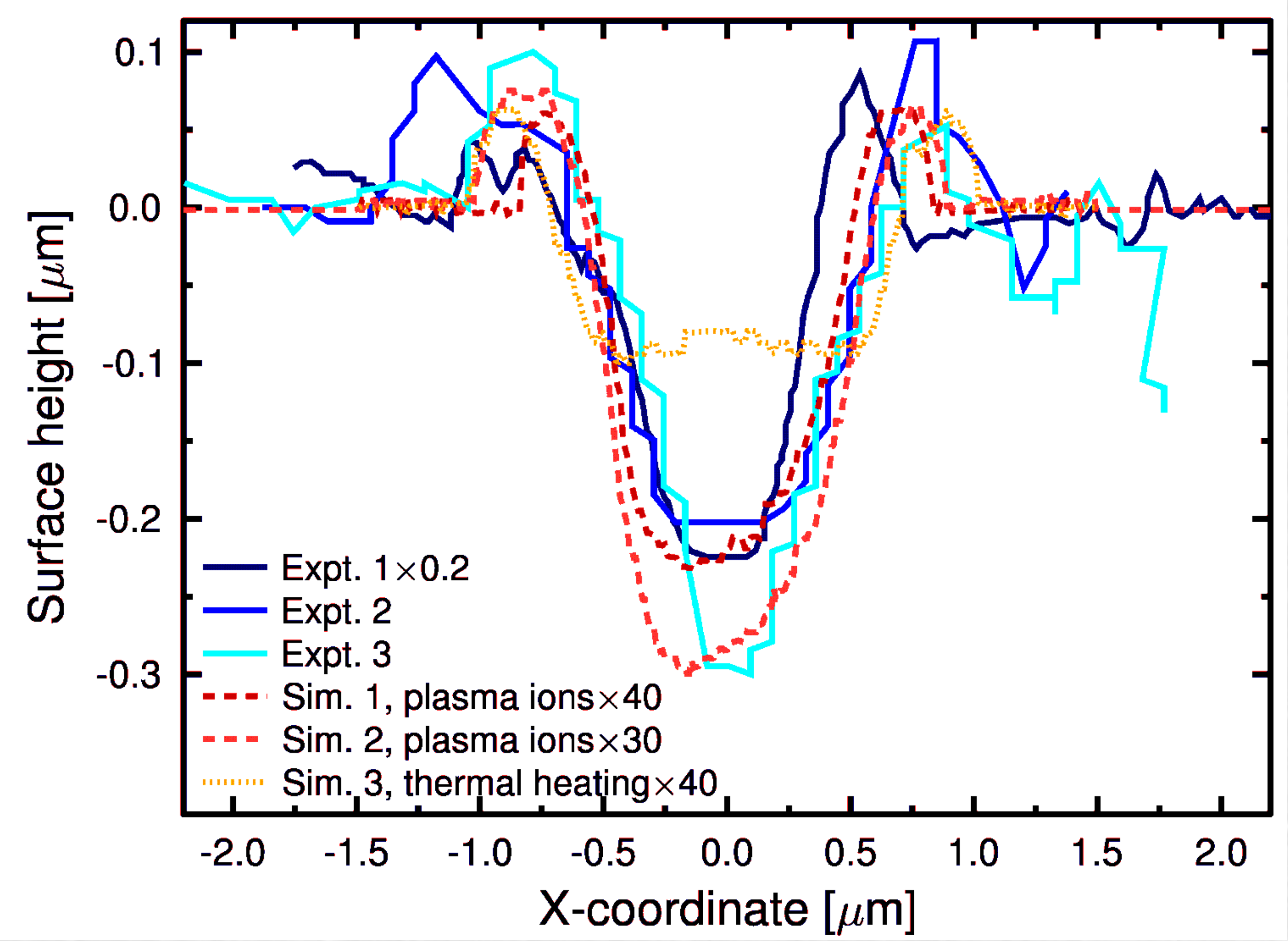


Comparison with experiments



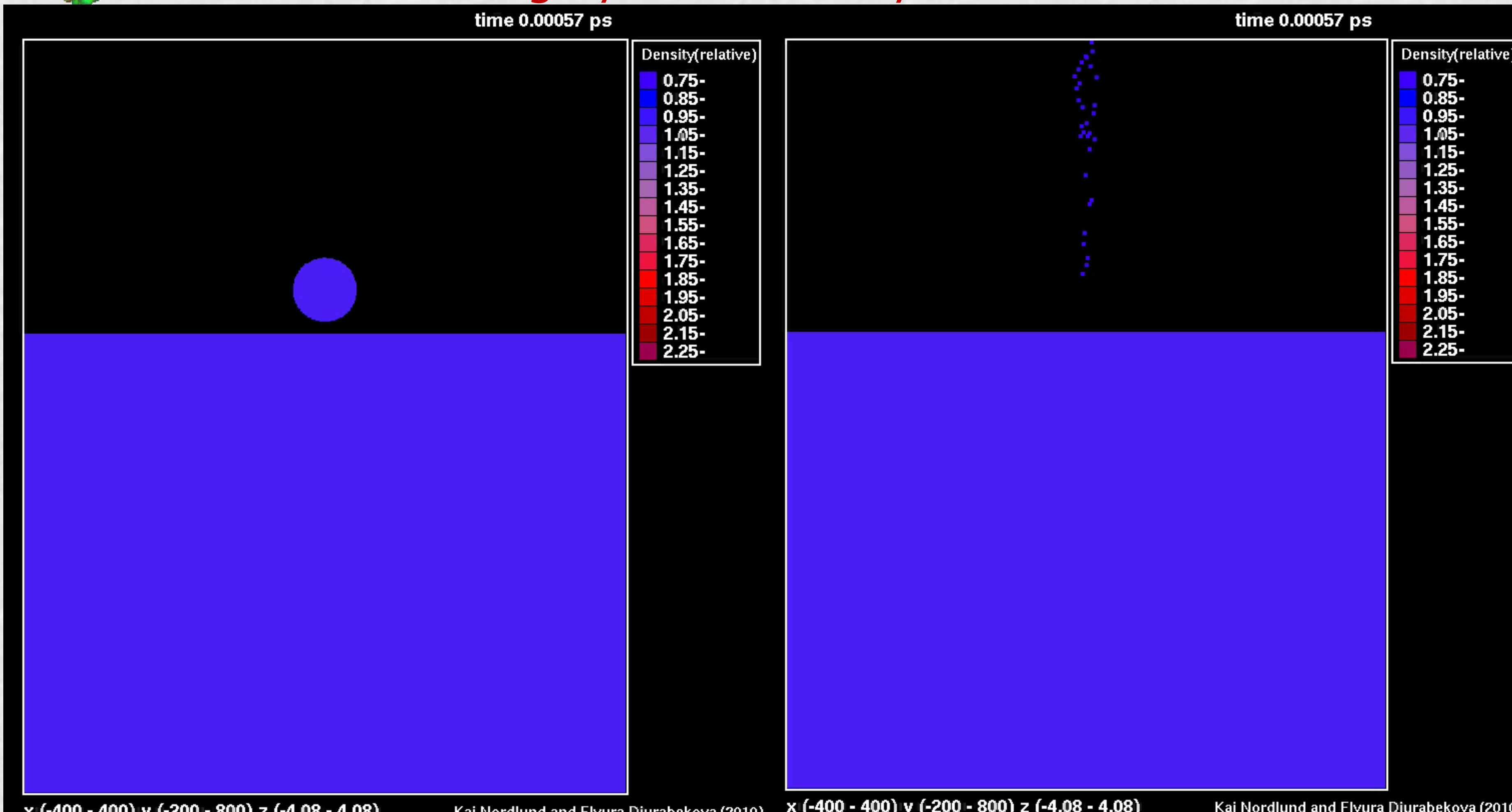
[Timko, Nordlund, Djurabekova et al, Phys. Rev. B 2009]

Comparison of shapes with experiments



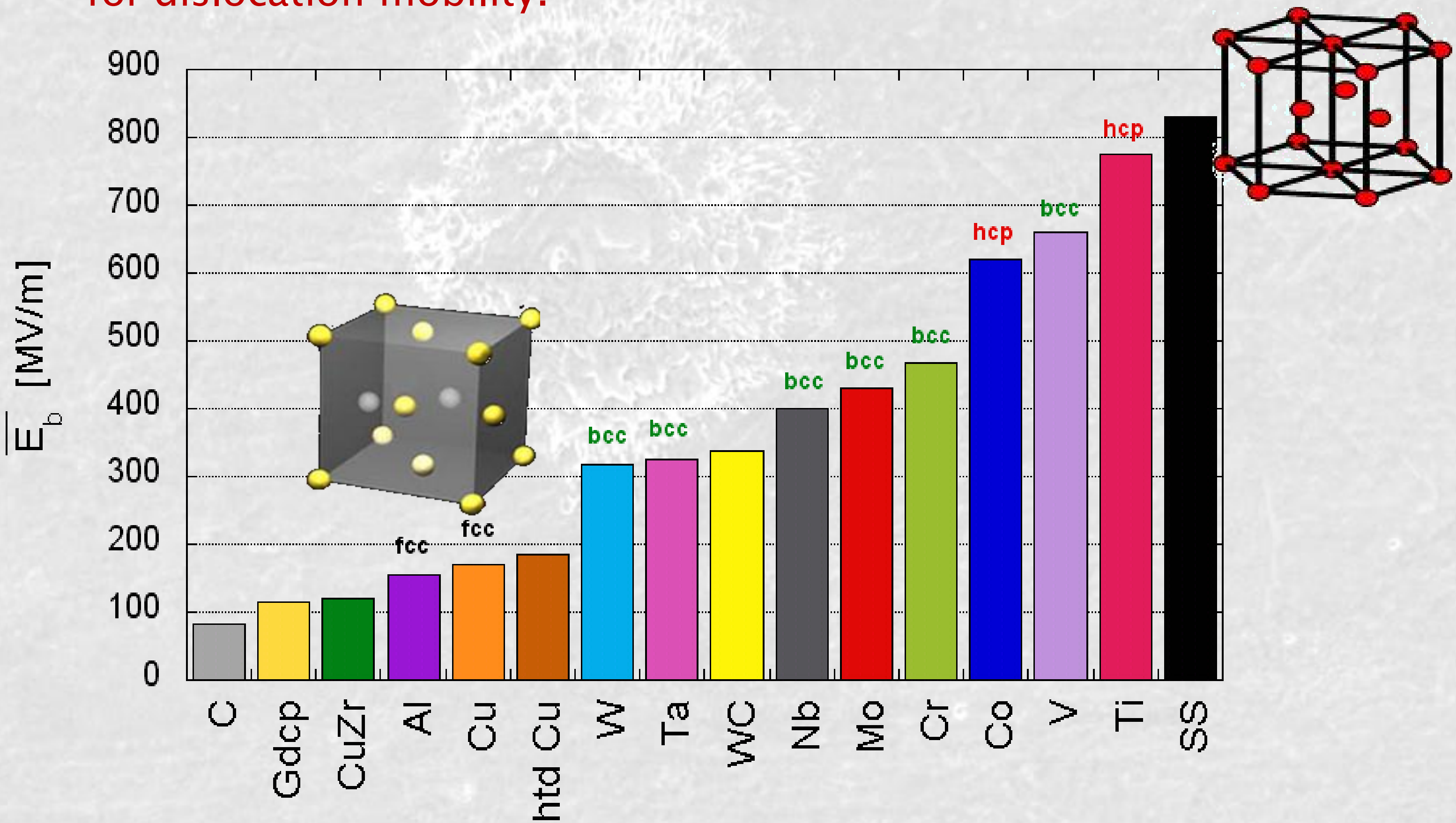
Stage 5: relation to cluster cratering?

- Cratering by cluster vs. by arc ions:



Experimental observation 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.



Dislocation mechanism of tip growth: why voids?

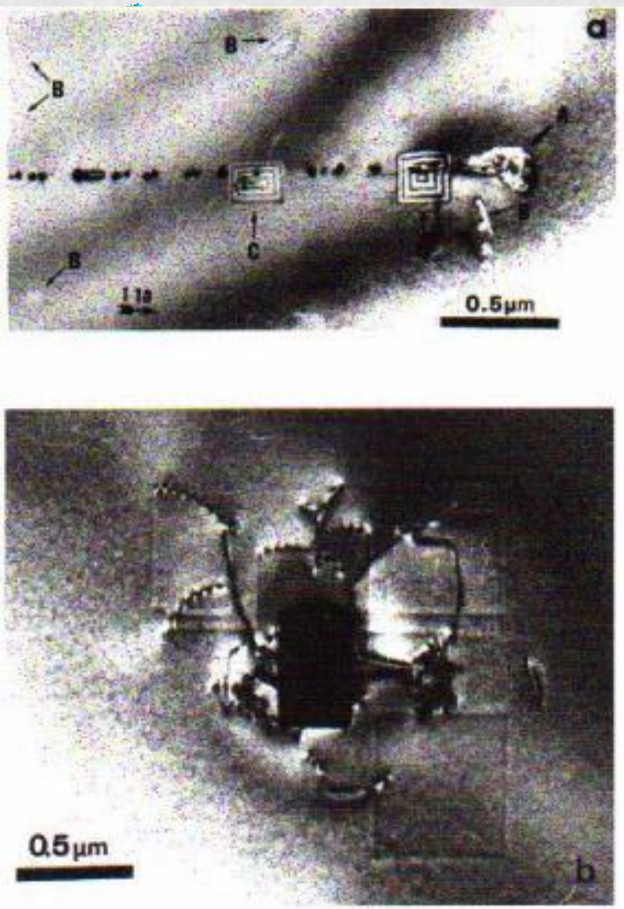
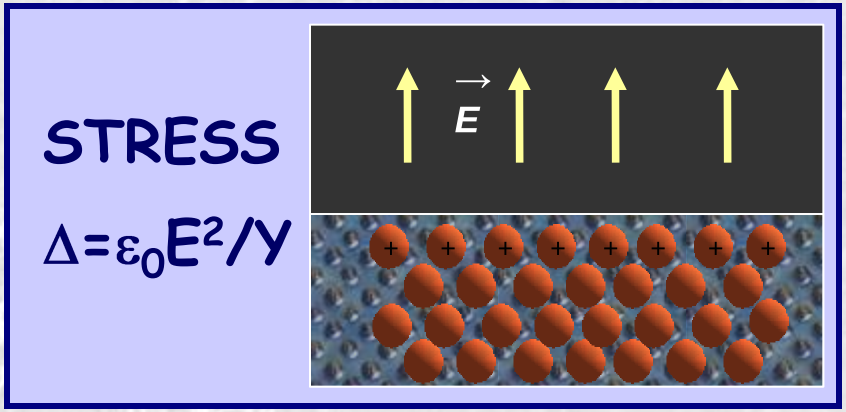
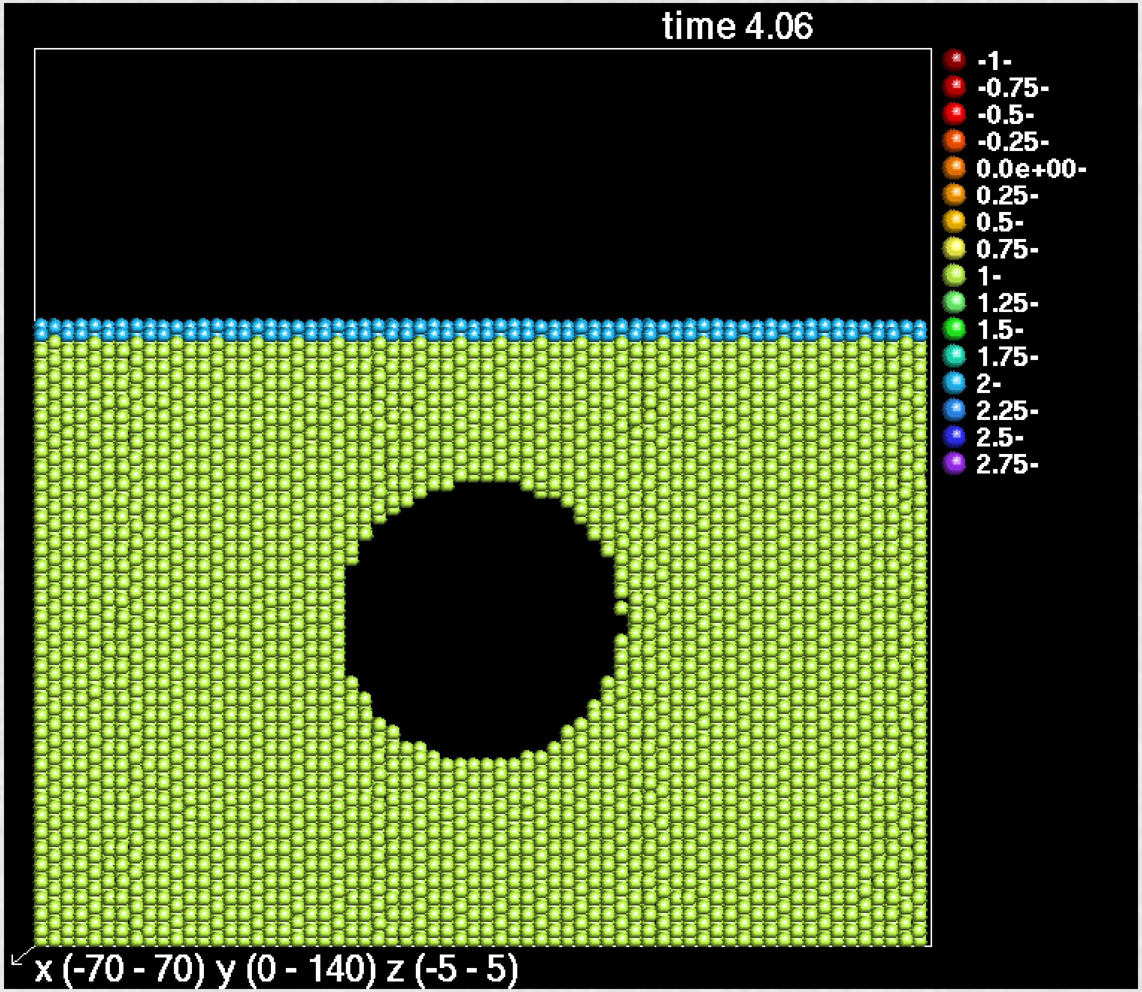


Figure 2:
TEM micrograph examples of copper (a) and nickel (b) precipitation induced disorder at wafer surfaces.



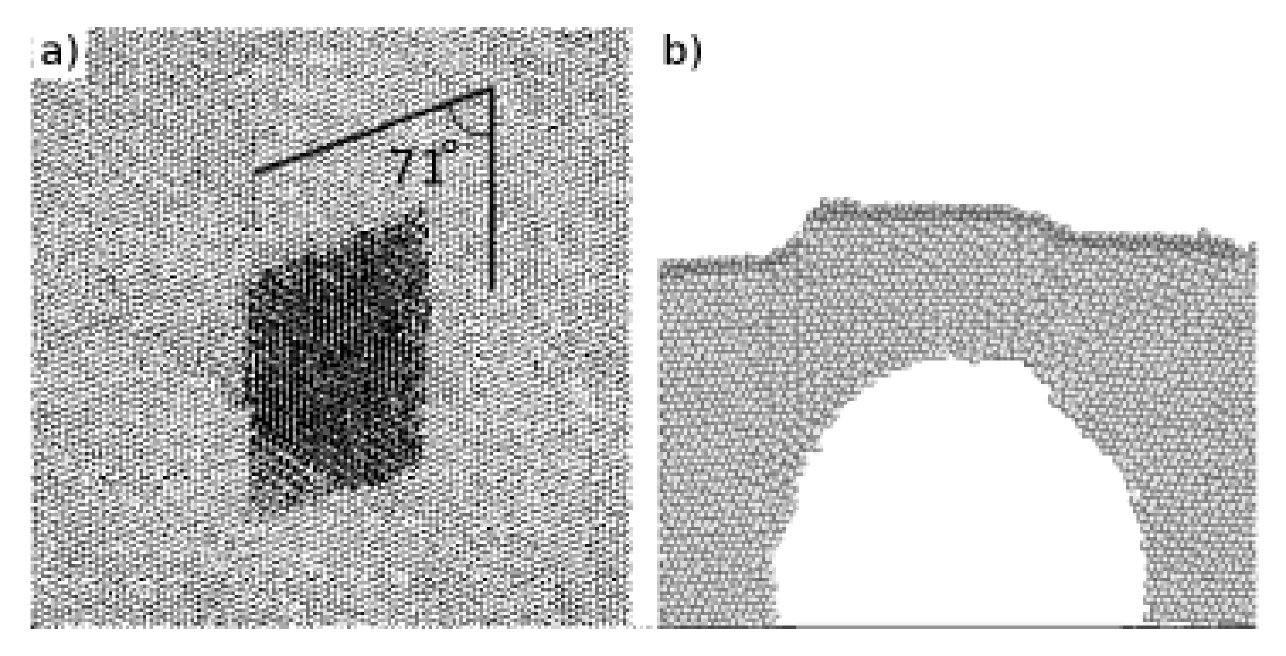
- In order to be able to form a stably growing structure, there is a need for a constant and consistent source of constructing pieces.
- The randomly distributed dislocations, which are always present in metals are not capable to build surface features due to the absence of repetitiveness.
- Any stress concentrator is a possible source of dislocation mechanism.
- We study one, which gives sufficiently plausible explanation for the origin of surface feature growth

Evolution of the surface held under tensile pressure (caused by electric field?)



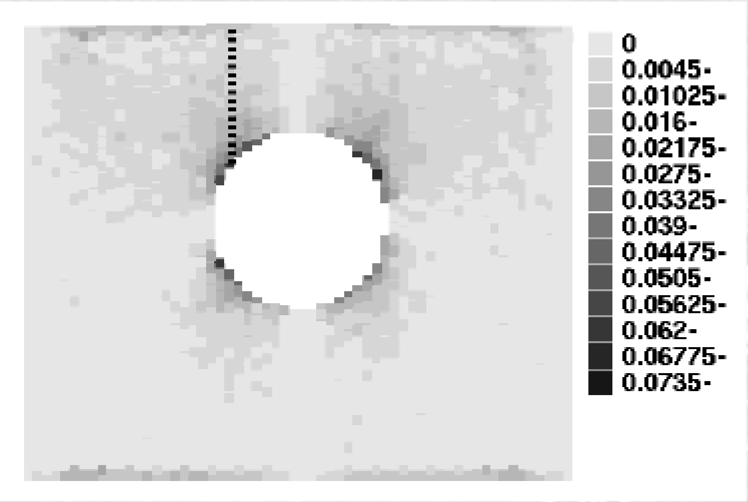
- If the tensile stress in order of several GPa is applied to the surface with the void, it eventually results in the protrusion on the surface

Dislocation mechanism for mass transport

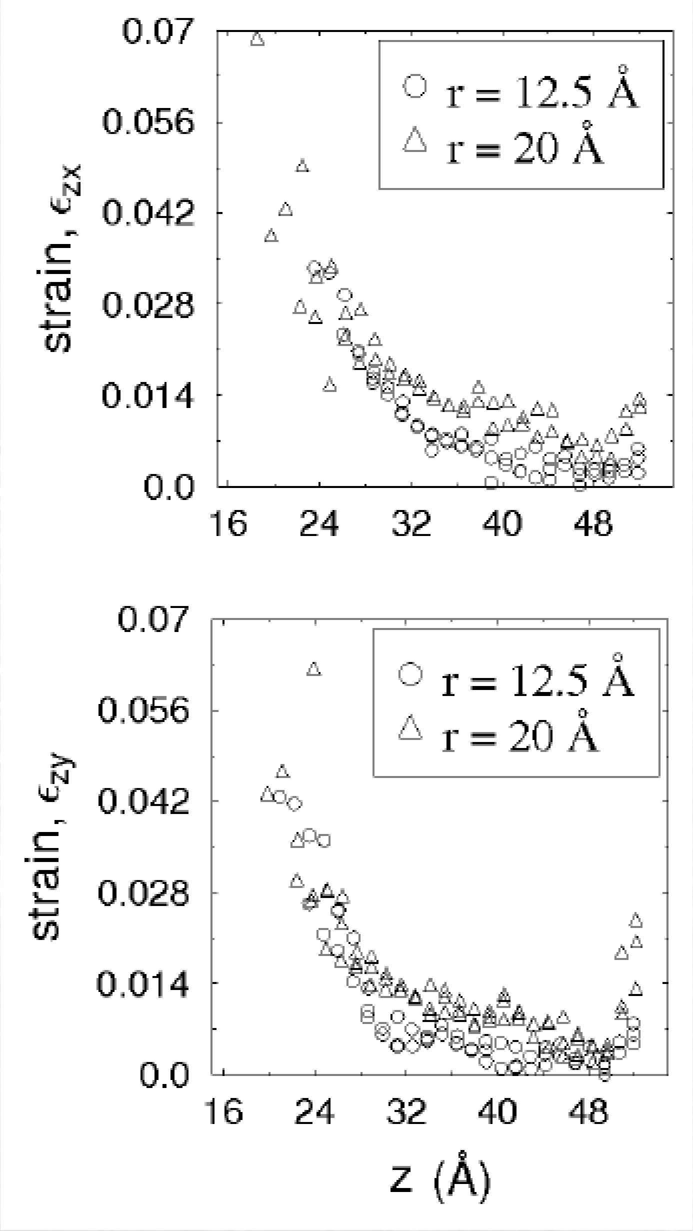


- The protrusion has a clear rhombic shape with the small angle 71°, which is the angle between two perpendicular to the surface {111} planes.

Strain calculation near the void



- The strain components ε_{zx} and ε_{zy} as a function of the z-coordinate of the atom. The atoms are analyzed along the path that starts at the most strained point on void surface and ends to the flat surface of the material.
- The void surface is at the lower end of the z coordinate value (18..24 Å).



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).

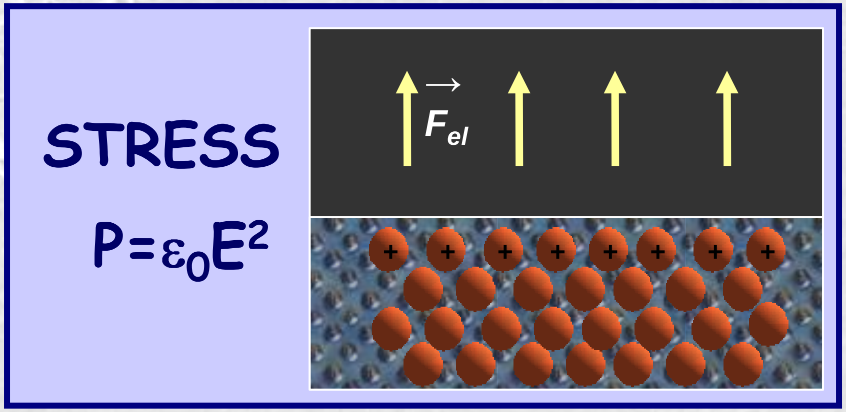
New interpretation to the old data:

- The concentration of defects in a material is* from standard thermodynamics

$$c = c_0 e^{-H^f/kT} = c_0 e^{-(E^f + P\Delta V)/kT}$$

where H^f if the formation enthalpy, E^f the formation energy and ΔV the formation volume of the defect. P is the pressure/stress exerted on the material.

- Now in the current case due to Gauss law the external electric field exerts a stress on the surface



* [Peterson, J. Nucl. Mater. 69 (1978) 3; Ehrhart, Properties and interactions of atomic defects in metals and alloys Landolt-Börnstein, New Series III ch. 2 p. 88-].

Electric field dependence

- Now assuming that the electric breakdown is caused by any defect mechanism, and the crucial step is nucleation of new defects due to the stress from electric field, it is reasonable to assume that breakdown rate $BDR \propto$ defect concentration c
- Moreover, the stress inside the material is of opposite sign to the external pressure. Hence one obtains:

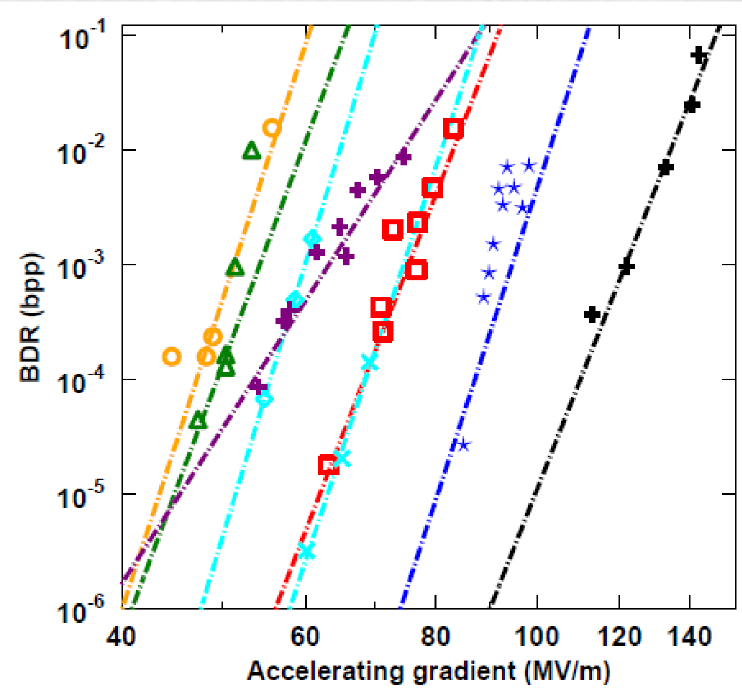
$$BDR \propto c = c_0 e^{-(E^f - \varepsilon_0 E^2 \Delta V)/kT} = c_0 e^{-E^f/kT} e^{\varepsilon_0 E^2 \Delta V/kT}$$

- Now grouping terms that are not dependent on the electric field and inserting a fitting prefactor A, this can be rewritten $BDR = A e^{\varepsilon_0 E^2 \Delta V/kT}$

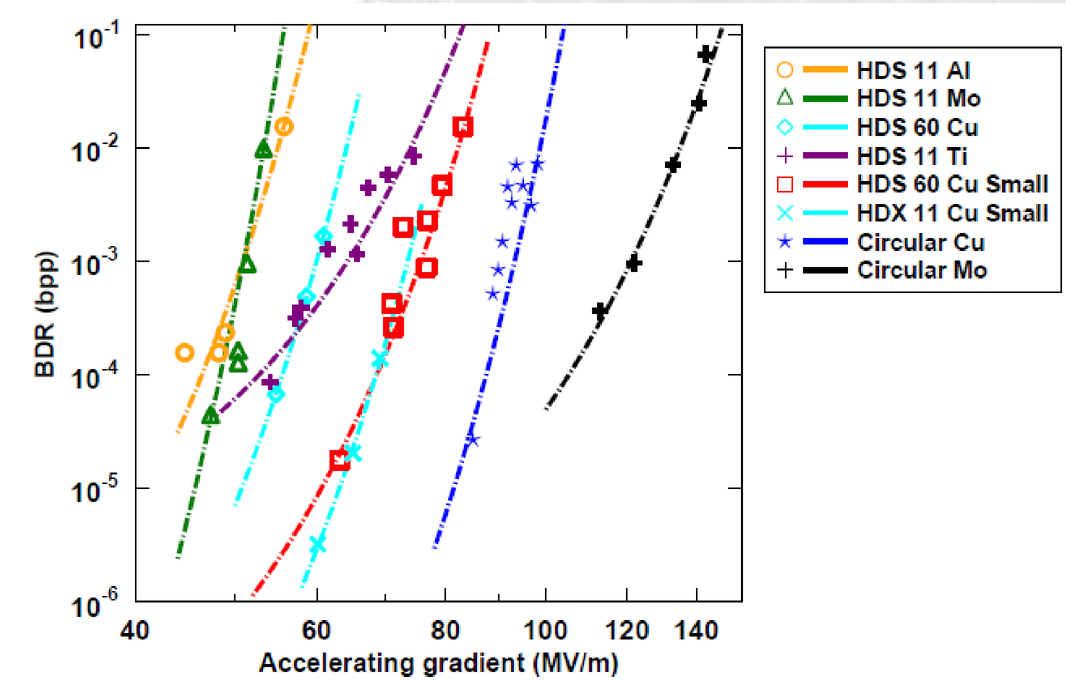
Electric field dependence

- Now to test the relevance of this, we fit the experimental data presented in [W. Wuensch, public presentation at the CTF3 collaboration meeting, Accelerating structure test results and what's next, available online at http://indico.cern.ch/conferenceDisplay.py?confId=8831.] with the model.] The result is:

Power law fit



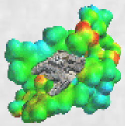
Stress model fit



Estimate of defect radius

- The ΔV term depends on the defect type and size, but is for interstitial-like defects of the order of the number of atoms in the defect times the atomic volume Ω.
- Our fits gave values of ΔV = 70 – 1100 nm^3 ≈7000 – 110000 Ω (Ω≈0.01 nm^3 for Cu).
- Now assuming circular prismatic interstitial-like dislocation loops (that can cause tip growth), and that each atom in a loop contributes 1 Ω to the relaxation volume (this is exactly true in the limit of very large dislocations) one can estimate the radius of one loop from $\pi r^2 d = \Delta V$, where d is the thickness of one atomic layer. Using d ≈ 0.2 nm one obtains a range of loop radii = 13 – 40 nm
- This is very reasonable compared to estimates of experimental loop sizes

Summary



- ✓ **We are developing a multiscale model to enable the better understanding of possible stages of evolution of an electrical breakdown phenomenon.**
- ✓ We initiated density functional theory calculations to calibrate the dynamic model ling of a charged metal surface as well as to investigate the modification of work function due to the presence of intrinsic defects on the surface.
- ✓ We also enabled the explicit account for the electronic dynamic in small protrusions on the surface to investigate the temperature effect in the probable nanoscale protrusions on the surface.
- ✓ We investigate the surface damage as a result of ion “shower” during the plasma discharge. The initial comparison with the experiment agrees with the linear scaling of experimental and simulated crater size
- ✓ We also suggest a new fitting law motivated by the dislocation activities in the surface layers.

Thank you!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