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HIP

Multiscale modelling of electrical breakdown at high-gradient electric field

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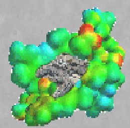
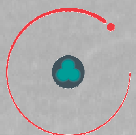
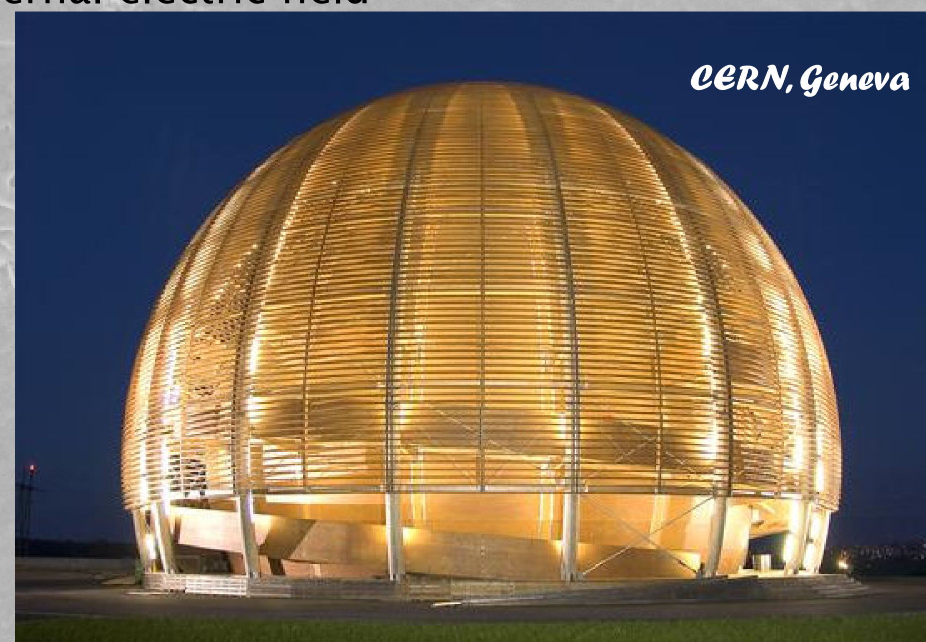
Outline



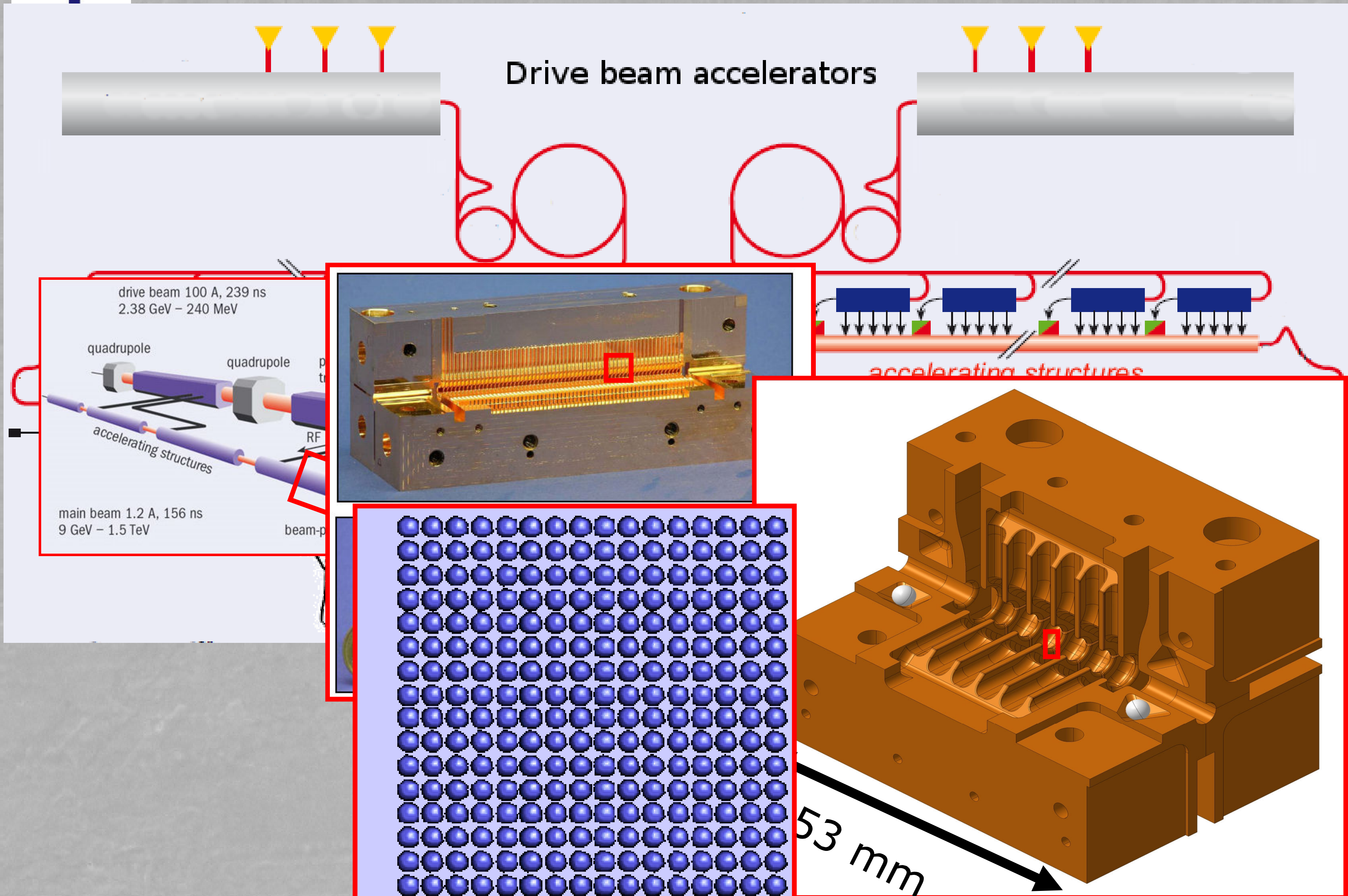
- Motivation: MD simulations for multi-km task?



- Multiscale model to approach the problem of electrical breakdown
  - Plasma onset due to the external electric field
  - Plasma simulation
  - Surface cratering
- Summary

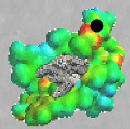


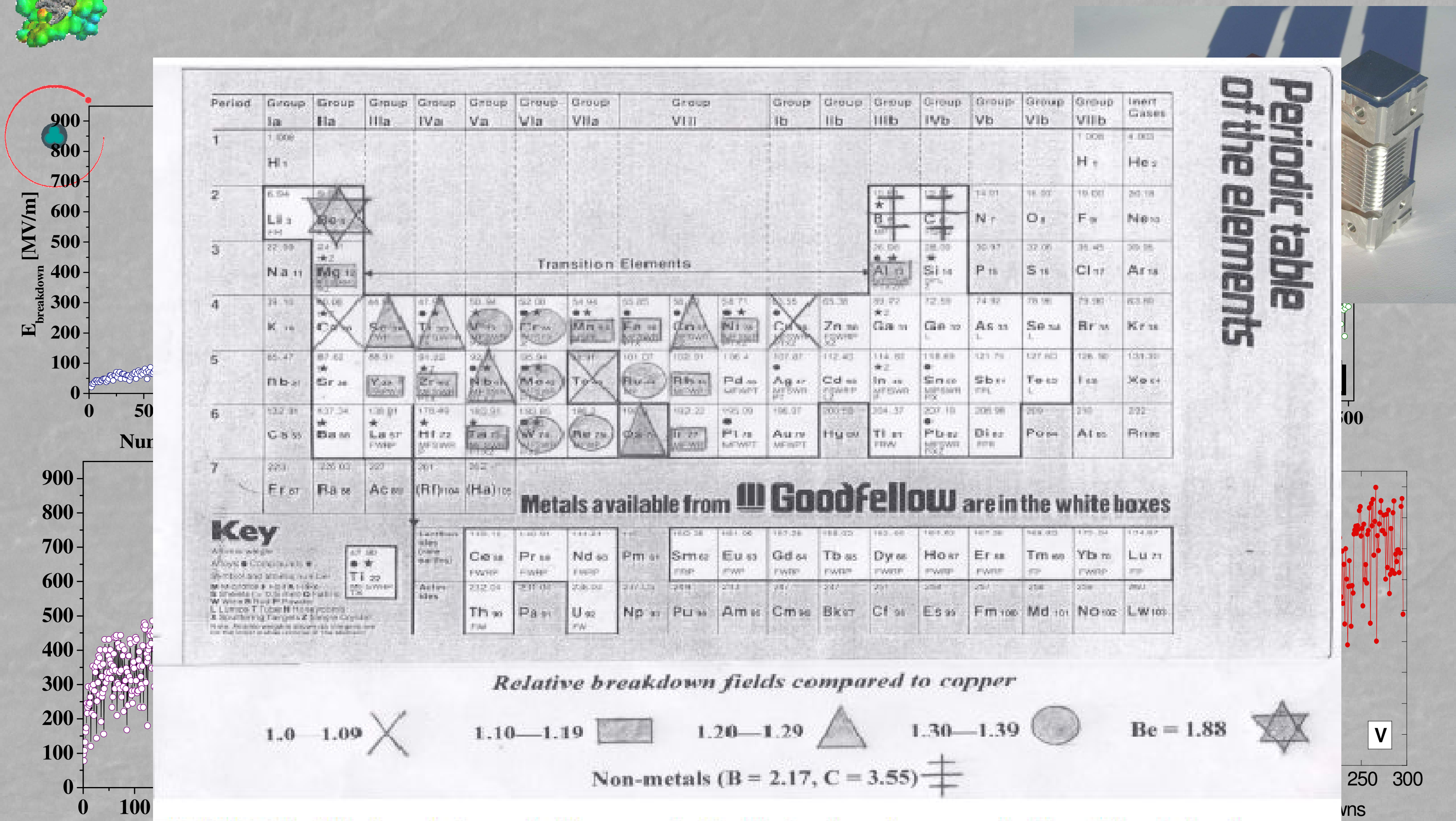
CLIC: "Compact" Linear Collider…



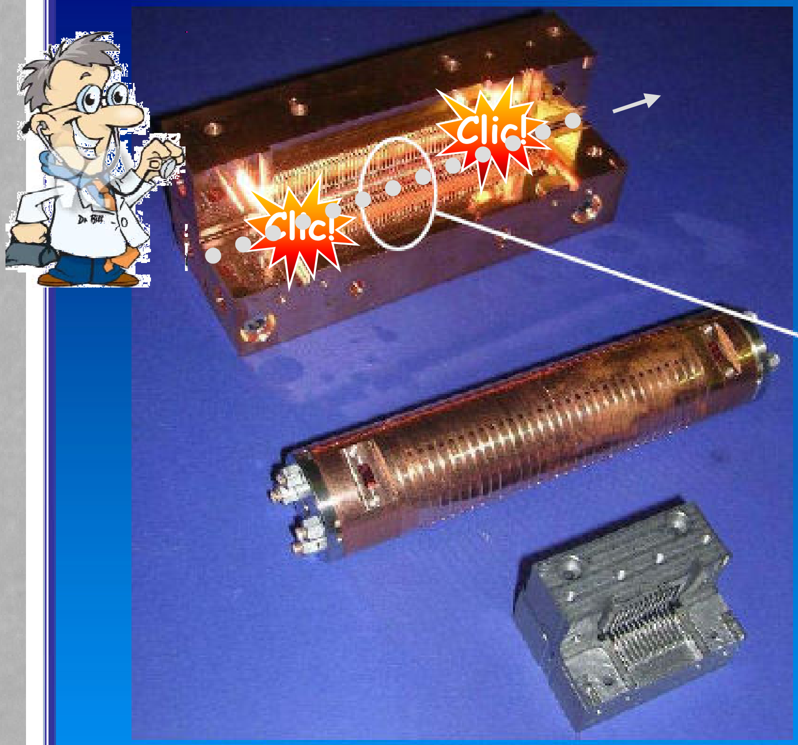
What we have learned at CLIC workshops…

S. Calatroni (2007),M.Taborelli(2007), P.Wilson (2006)

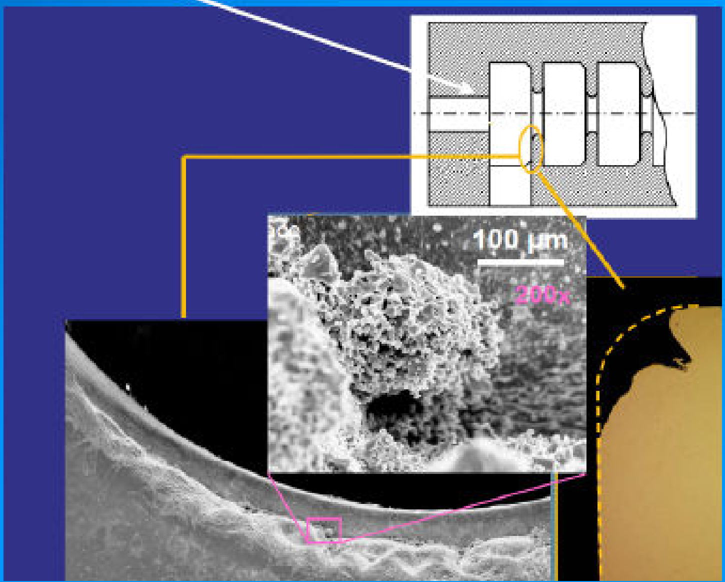




Detecting the problem…

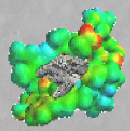


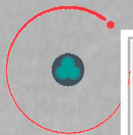
100-150
MV/m



Rf-accelerating structures for CLIC and damage observed during the operation.

Electrical Breakdown in multiscale modeling approach





Stage 0: Onset of tip growth; Dislocation mechanism
Method: MD, Molecular Statics… — ~ sec/min

Stage 1: Charge distribution @ surface
Method: DFT with external electric field — ~few fs

Stage 2: Atomic motion & evaporation
Method: Hybrid ED&MD model — ~few ns

- Classical MD+Electron Dynamics: Joule heating, screening effect
- Solution of Laplace equation

Stage 3: Evolution of surface morphology due to the given charge distribution
Method: Kinetic Monte Carlo — ~ sec/hours

=> Electron & ion & cluster emission ions

Stage 4: Plasma evolution, burning of arc
Method: Particle-in-Cell (PIC) — ~10s ns

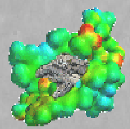
=> Energy & flux of bombarding ions

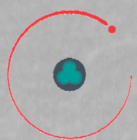
Stage 5: Surface damage due to the intense ion bombardment from plasma
Metod: Arc MD — ~100s ns

PLASMA ONSET

Our basic technique: Molecular dynamics

Simulating atom motion:





Give atoms initial $\boldsymbol{r}^{(t=0)}$ and $\boldsymbol{v}^{(0)}$, choose short Δt

↓

Get forces $\boldsymbol{F} = -\nabla V(\boldsymbol{r}^{(i)}) + \boldsymbol{F}_{el}$ *or* $\boldsymbol{F} = \boldsymbol{F}(\Psi)$ and $\boldsymbol{a} = \boldsymbol{F}/m$

↓

Move atoms: $\boldsymbol{r}^{(i+1)} = \boldsymbol{r}^{(i)} + \boldsymbol{v}^{(i)}\Delta t + {}^{1}/_{2}\,\boldsymbol{a}\,\Delta t^2$ + correction terms

Update velocities: $\boldsymbol{v}^{(i+1)} = \boldsymbol{v}^{(i)} + \boldsymbol{a}\Delta t$ + correction terms

↓

Move time forward: $t = t + \Delta t$

↓

Repeat as long as you need (→ back to "Get forces")

Plasma onset

Stage 0: Onset of tip growth; Dislocation mechanism

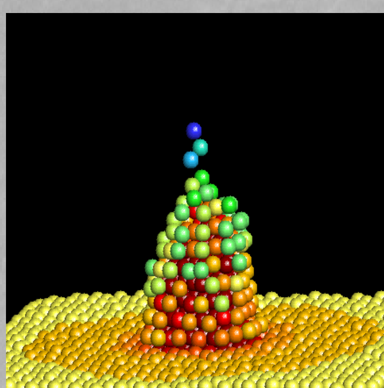
Method: MD, Molecular Statics…

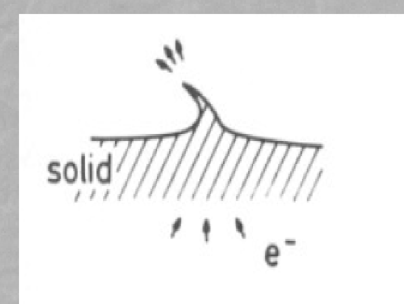
↓

Stage 2: Atomic motion & evaporation

Method: Hybrid ED&MD model

- Classical MD+Electron Dynamics: Joule heating, screening effect
- Solution of Laplace equation





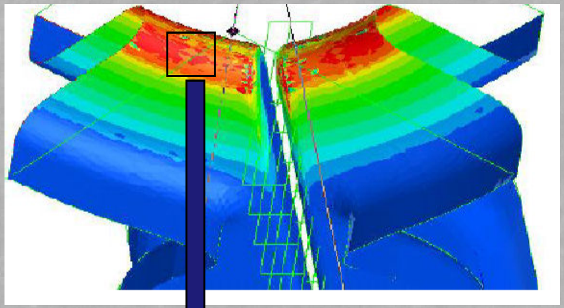
External electric field: classical electrodynamic approach

Gauss law states

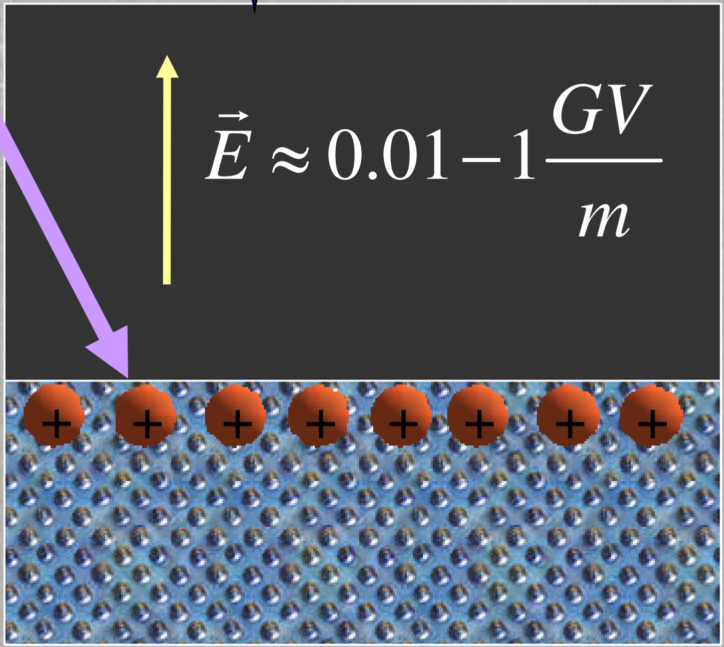
$$\sigma = \frac{Q_{surface}}{A_{surface}} = \varepsilon_0 E$$

Due to the external electric field the surface attains charge

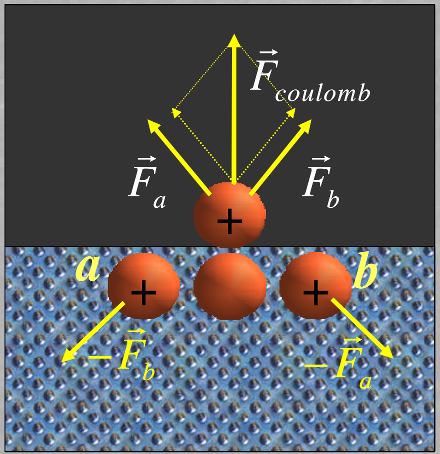
Macroscopic field to…



…the atomic level:



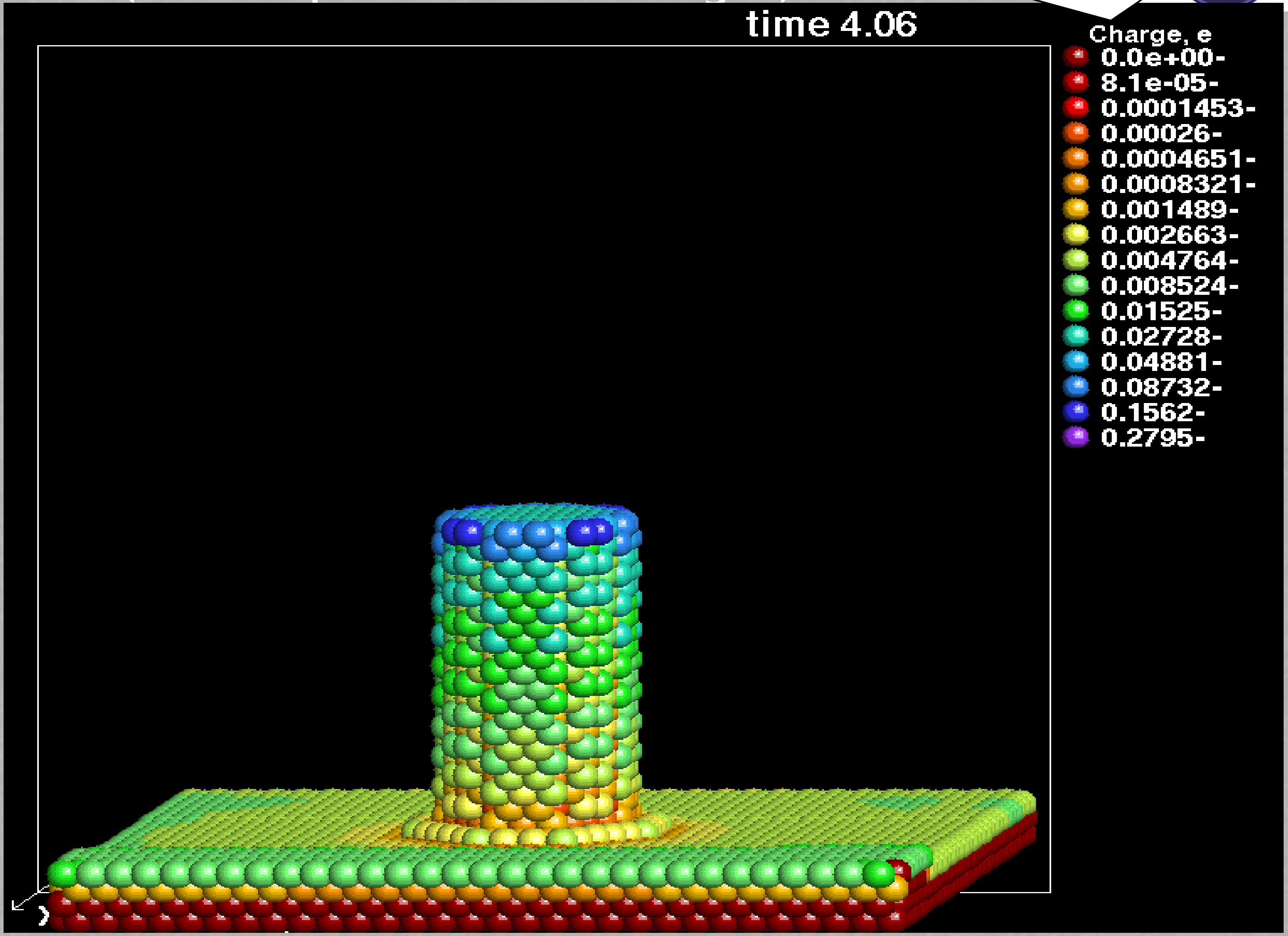
Two electric forces modify the motion of charged atoms:



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

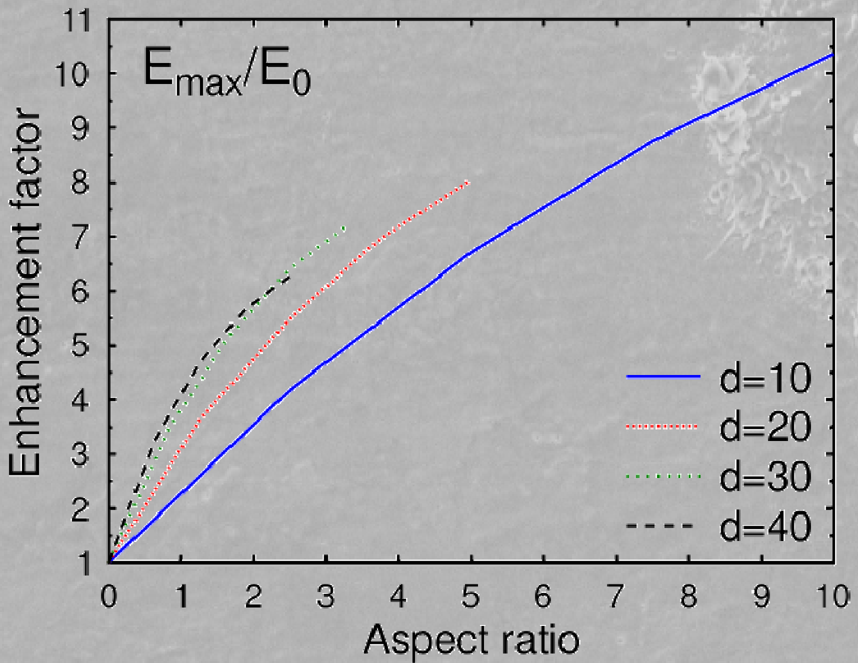
$$\vec{F}_C = \frac{1}{4\pi\varepsilon_0}\sum_i \frac{q_a q_i}{r_{0i}^2}\hat{r}_{0i}$$

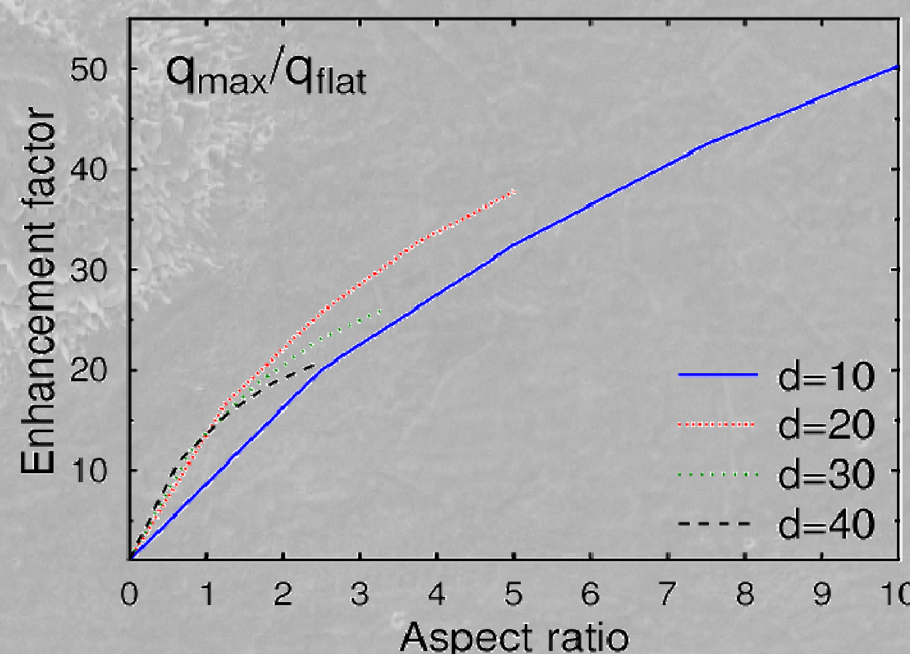
Solution of 3d Laplace equation for the surface with the tip of 20 atomic layers (color represents the charges)



Results of static calculation of charge distribution on atoms

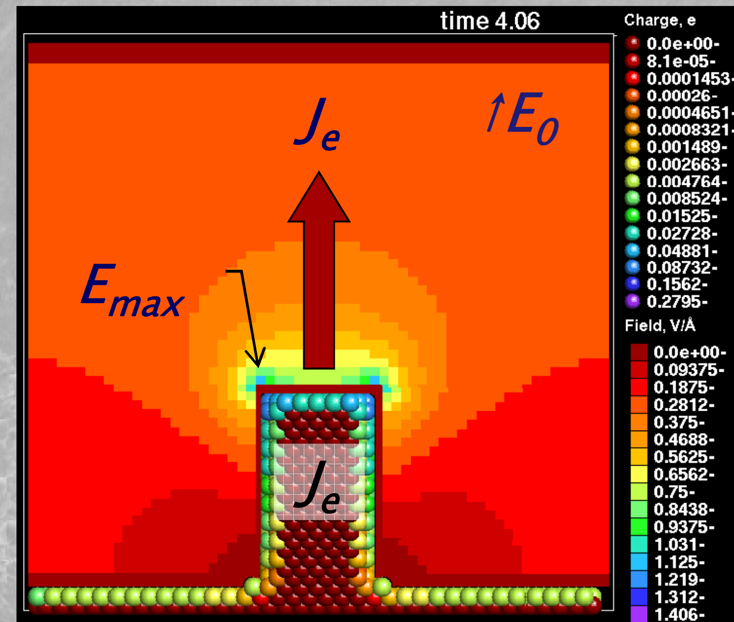
- The thinnest tips show the closest to linear proportionality between the hight and enhancement factor as observed in experiment

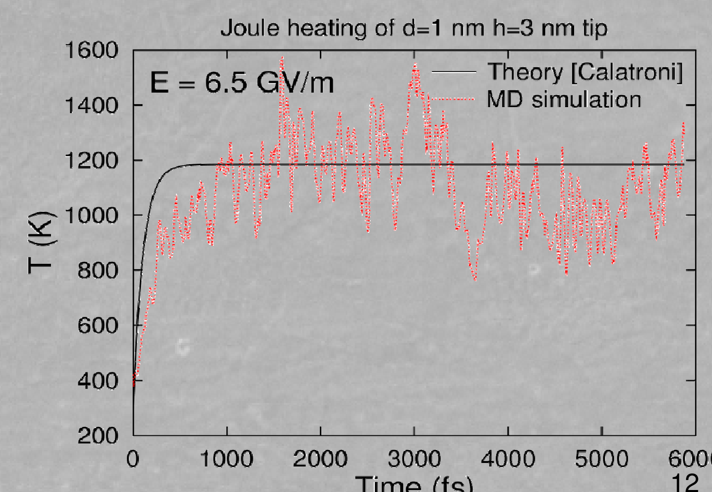




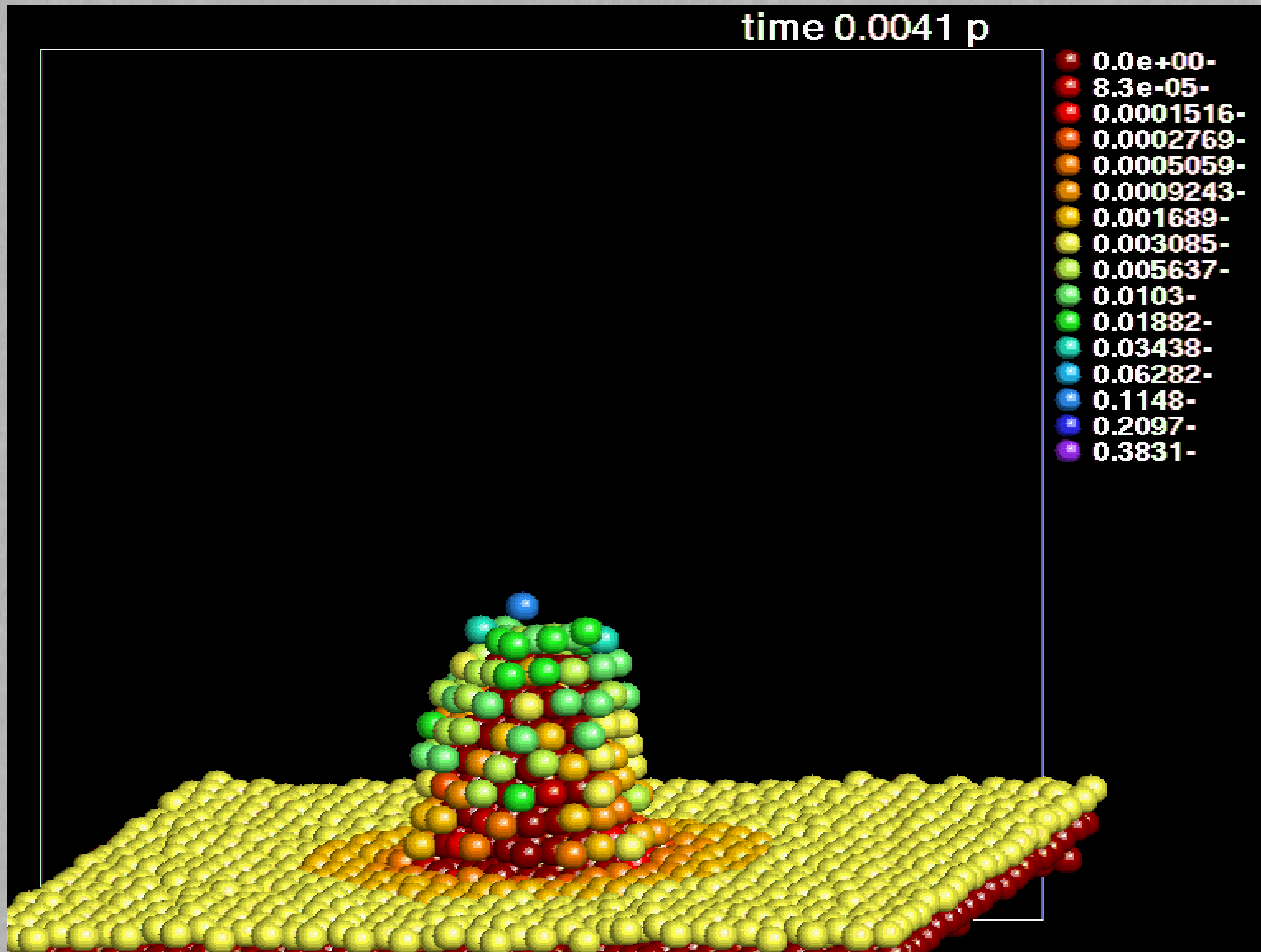
Implementation of Joule heating

- The enhanced Fowler-Nordheim electron emission from sharp tips leads to a strong electron current J_e through the tip
- This in turn will lead to a Joule heating of the tip
- We have implemented Joule heating of the tip
  - Stochastic additional velocities given to atoms corresponding to the heating rate from Ohms law

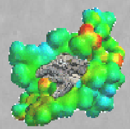


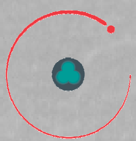


Atom/cluster evaporation from Cu(100) @ 500 K, E_0 = 1 GV/m

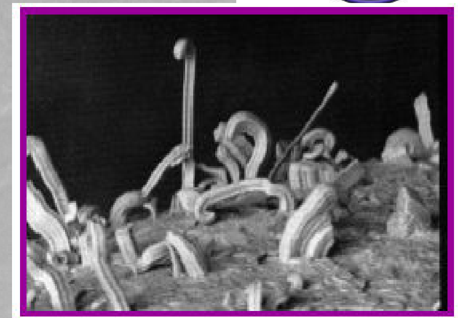


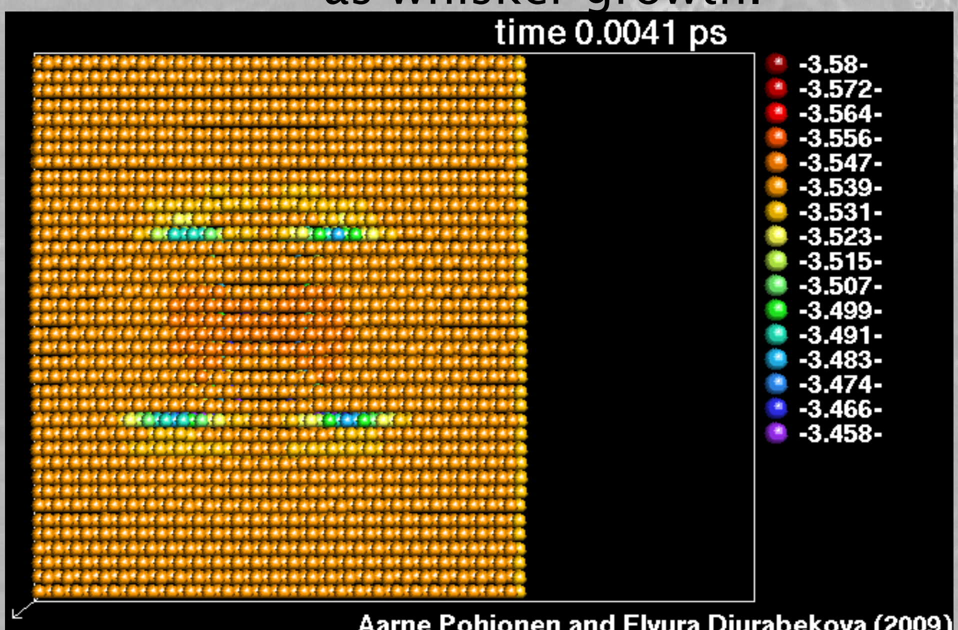
But… We still must explain why the growth is possible?

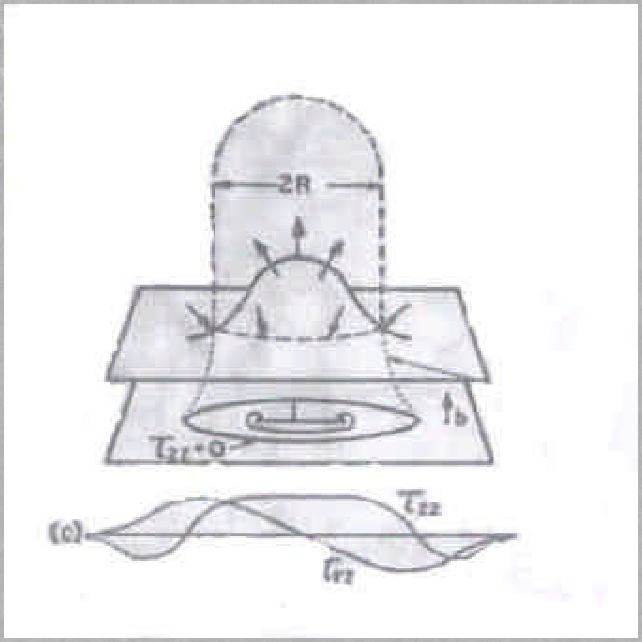




- Looking for the plausible explanation of surface roughening and possible mechanisms we found an interesting fact: there is a large field of research on such a mysterious phenomenon as whisker growth.

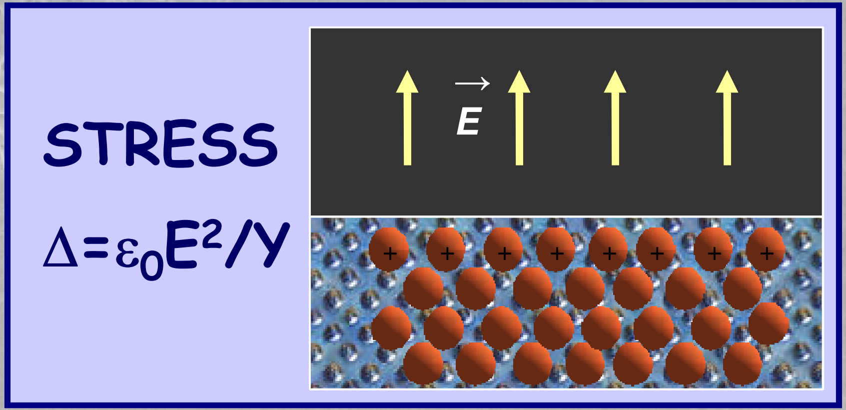






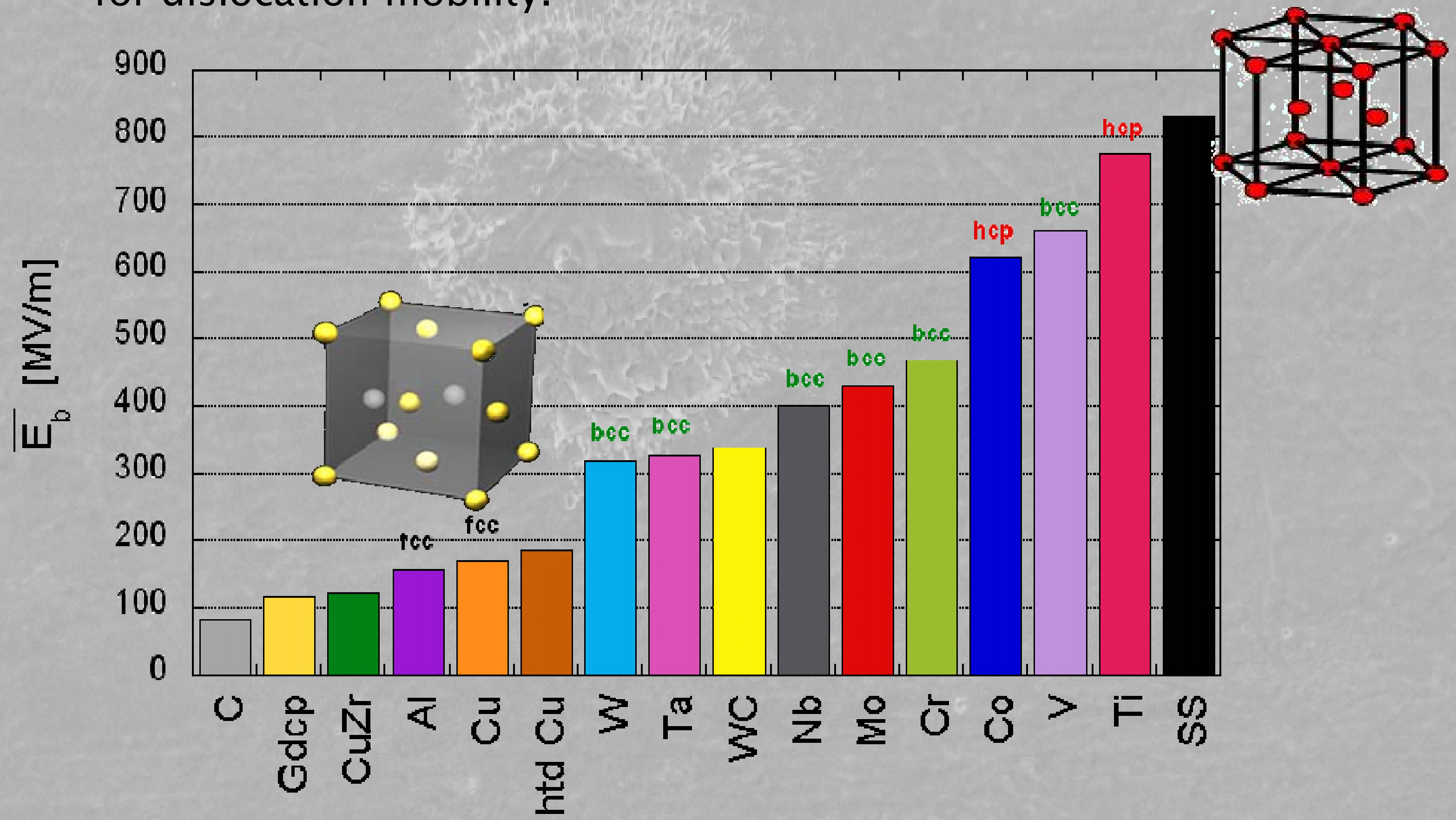
Stresses due to the field

- The main agreement in the field is that the rapid releasing of microstresses, which is generally present on grain boundaries and can be enhanced by any external agents as mechanical treatment or T-cycling, the migration of defect complexes is stimulated.
- The strain by the huge electric field can cause the dislocation motion and redistribution of the microstress.

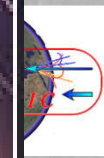


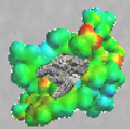
Recent experiment at CERN: CLIC-note

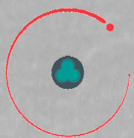
- The dislocation motion is strongly bound to the atomic structure of metals. In FCC (face-centered cubic) the dislocation are the most mobile and HCP (hexagonal close-packed) are the hardest for dislocation mobility.



Plasma



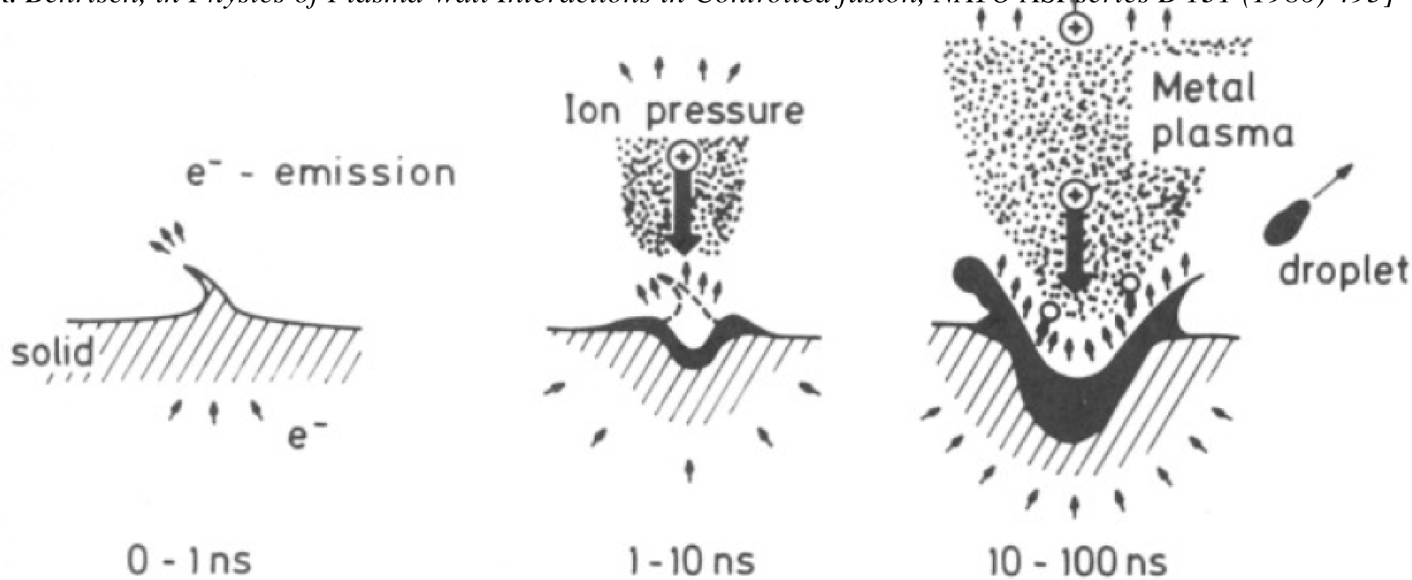




Stage 4: Plasma evolution, burning of arc
Method: Particle-in-Cell (PIC)

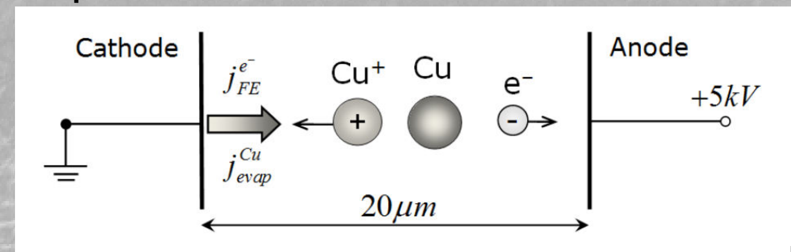
~10s ns

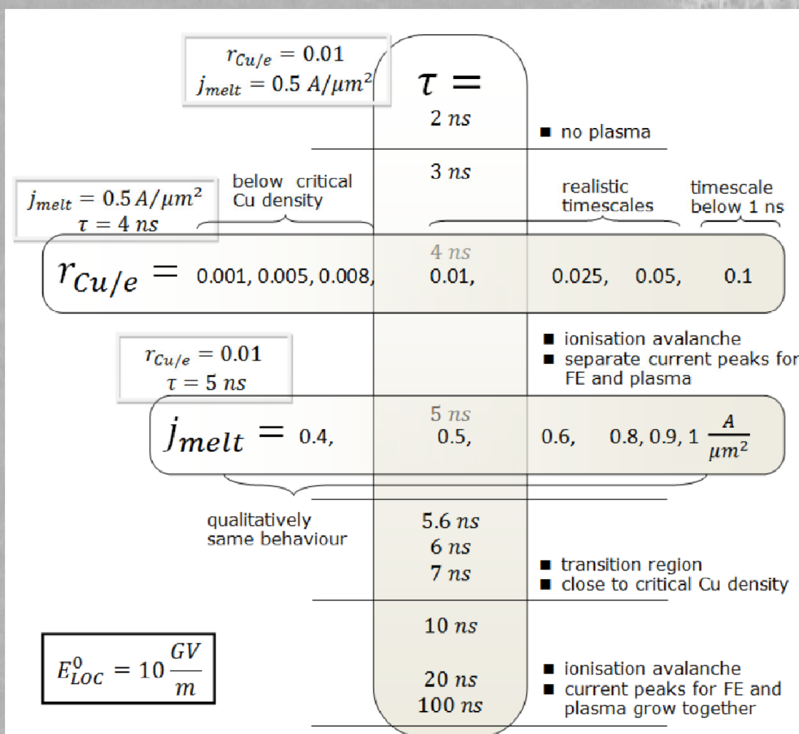
[R. Behrisch, in Physics of Plasma-wall Interactions in Controlled fusion, NATO ASI series B 131 (1986) 495]



Plasma simulations in collaboration with CERN (S.Calatroni) (cf. talk at by H.Timkò, WG4 15.10: 14:00)

- 1d Particle-in-Cell (PIC) plasma simulation has been developted to describe the development of the arc plasma after the onset.
- Parametrized from experiment and MD simulations

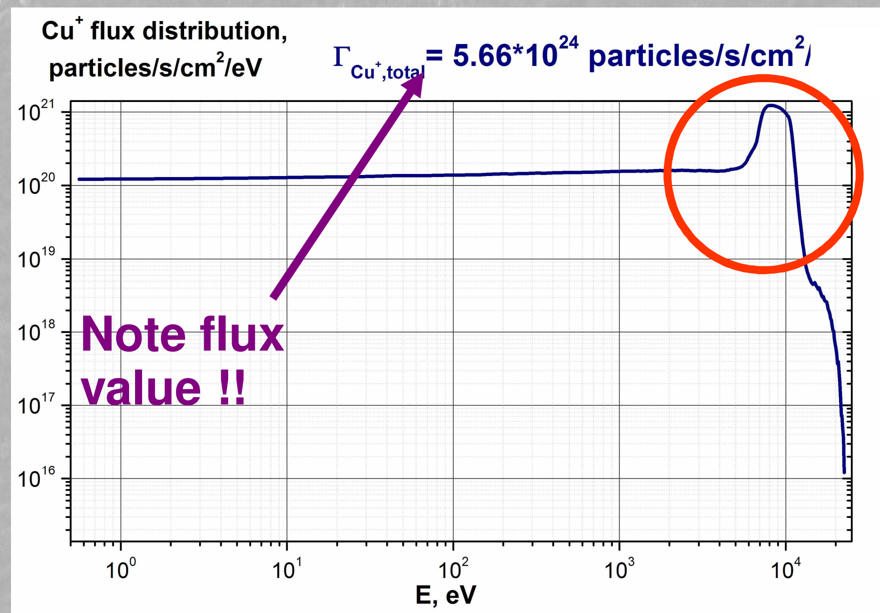




As a result we show a diagram of combinations of DC setup decay time constant τ, electric field *E*, melting current *j* and Cu to e evaporation ratio r_{Cu}/e lead to electric breakdown. Results are waiting for approval to be submitted.

Surface damage while arcing

- The PIC simulations gave particle flux and energies due to plasma sheath potential

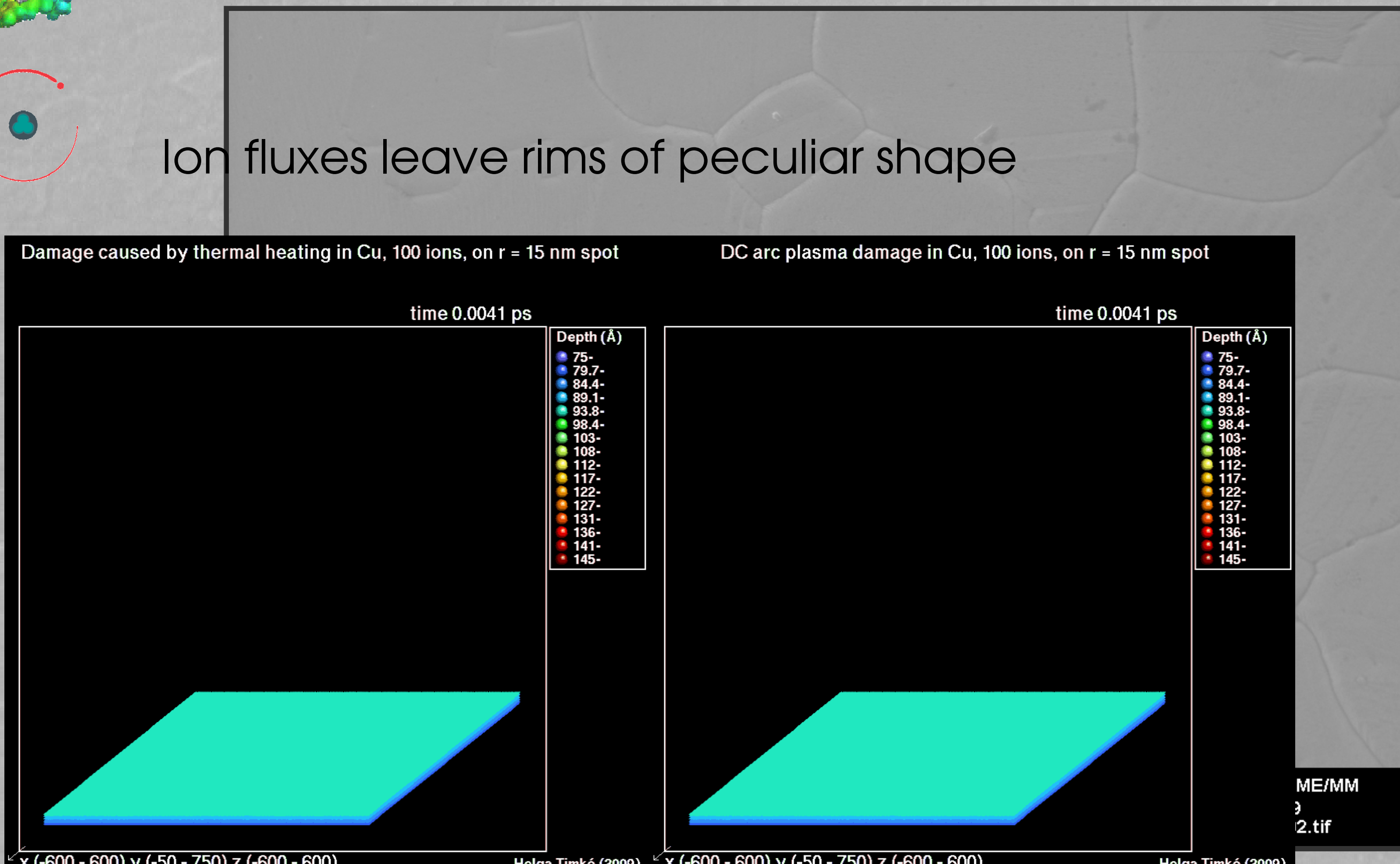


Stage 5: Surface damage due to the intense ion bombardment from plasma
Metod: Arc MD

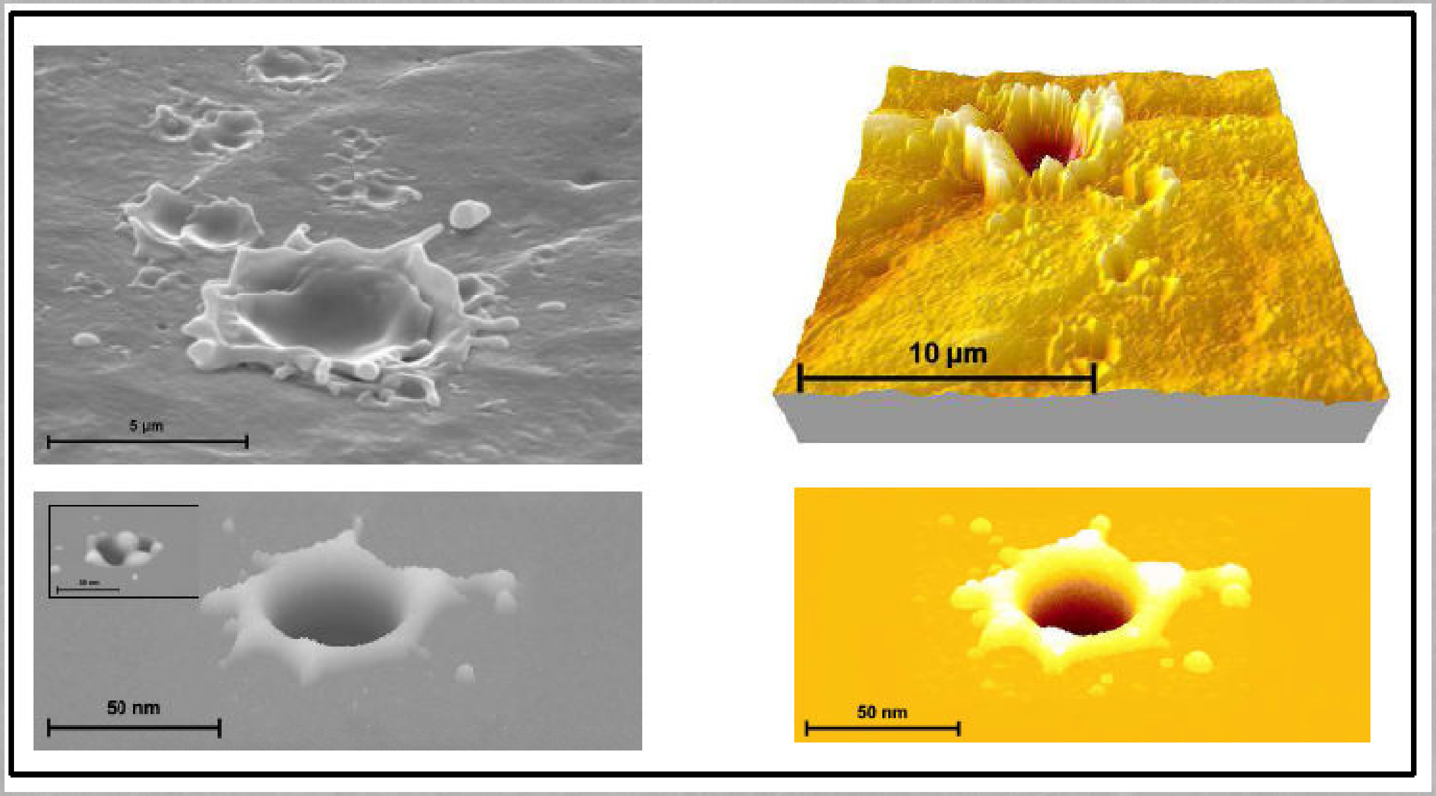
~100s ns

Huge fluxes of accelerated ions are the reason for surface damage

Ion fluxes leave rims of peculiar shape



AFM measurements of single spark event produced at CERN

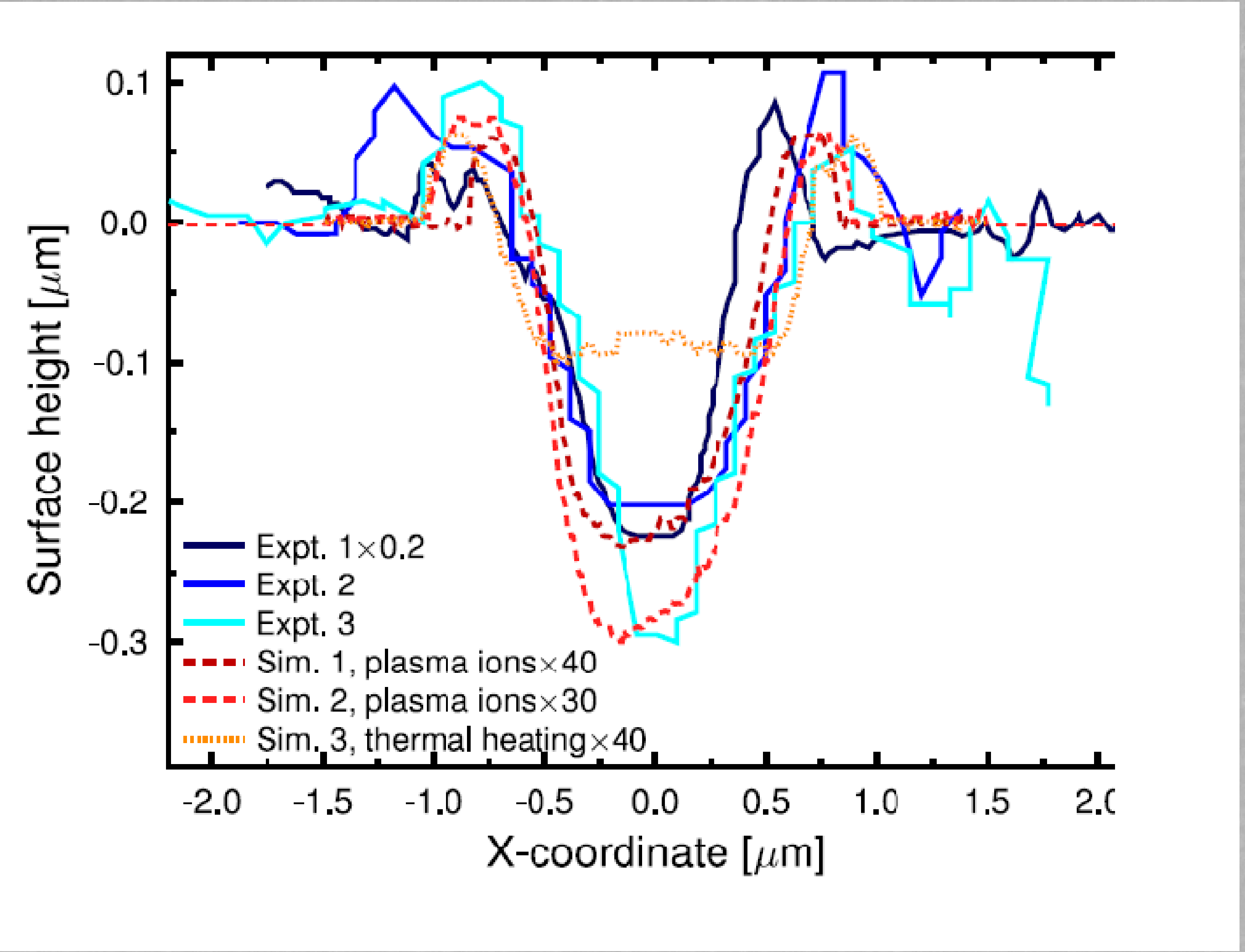


Top left: tilted SEM image (CERN)

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 simualtion (submitted for publication)



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’s motions

Thank you!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