Fundamentals of metal surfaces behavior under high electric fields

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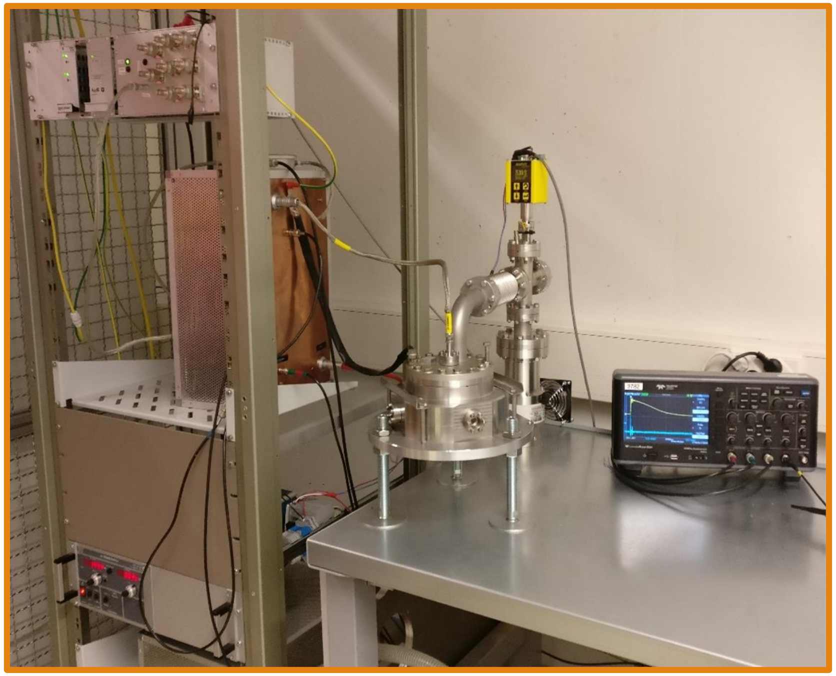
A new home for LES @ Helsinki: Current status by A. Saressalo

LES has recently been transferred to the Accelerator laboratory at University of Helsinki (MSc Anton Saressalo)

Now we are ready to run our own experiments.

Current status:

- All the devices have been installed
- Signal Transceiver and Quad Bus Buffer chips replaced in the High Rep Rate Controller
- Turbo pumped vacuum close to UHV and improving (< 5 x 10-9 mbar)
- LabVIEW program almost completely redesigned
- Still follows the same conditioning algorithm as at CERN
- Threshold voltages calibrated to detect the breakdowns from normal pulses
- Able to run several pulsing periods (e.g. 105 pulses), detect BD's and continue the algorithm
- Yet still difficulties with longer runs

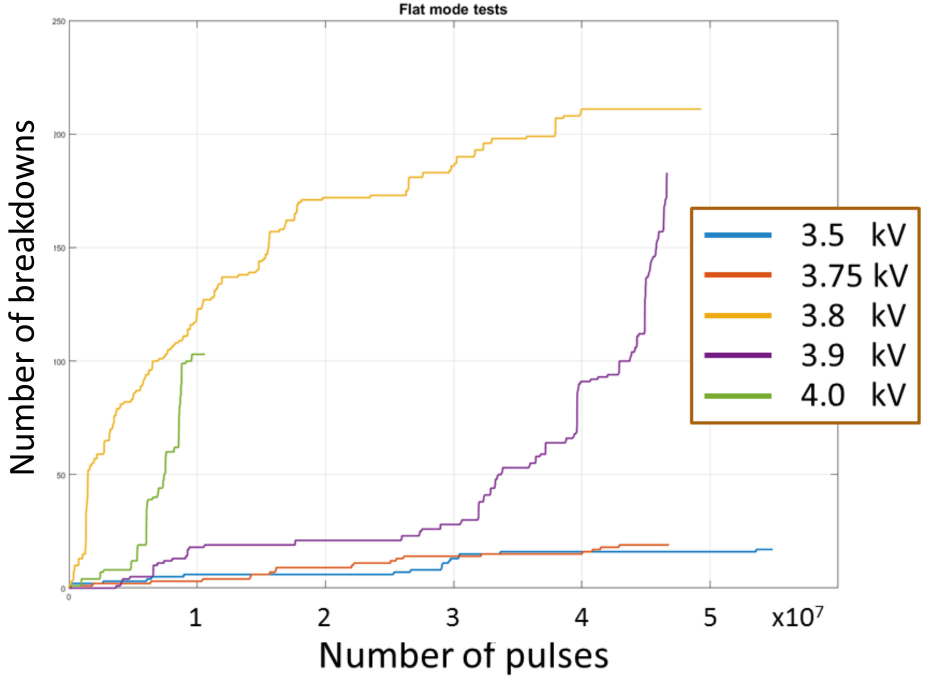


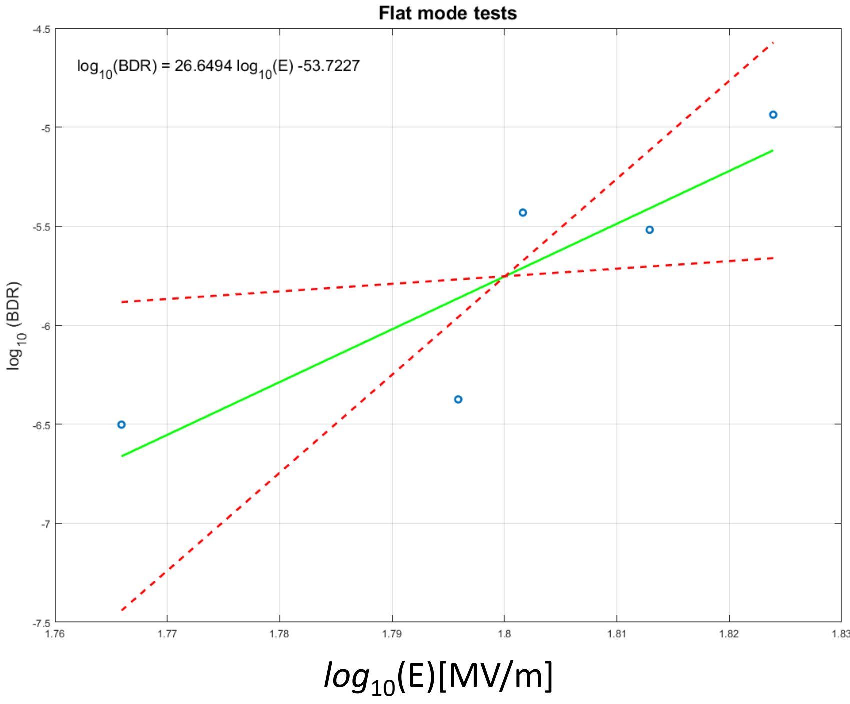
Experimental results from Helsinki

First runs in the flat mode resulted in the following:

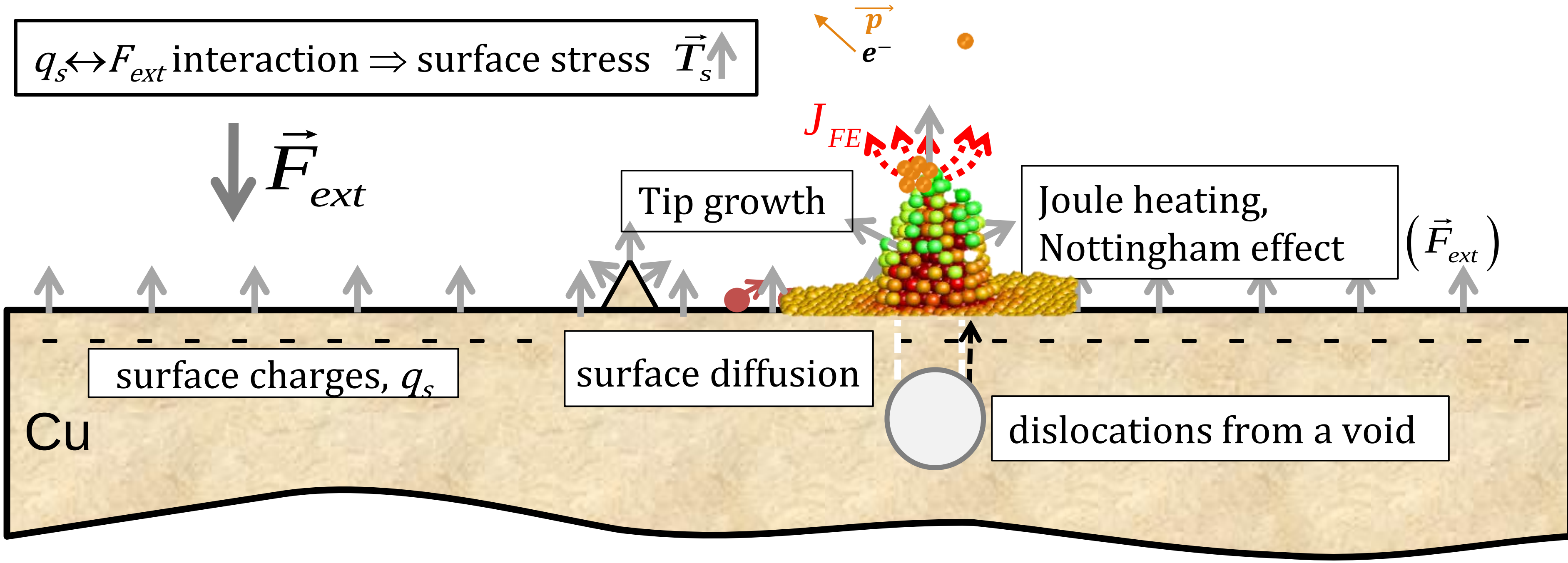
By using formula:

$$\frac{E^{\alpha}\tau^{\beta}}{BDR} = A$$





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



Electronic effects in MD

General agreement:

- Electron emission initiates vacuum arcs.

However, the *exact mechanism* is still unclear.

Fundamental question to answer:

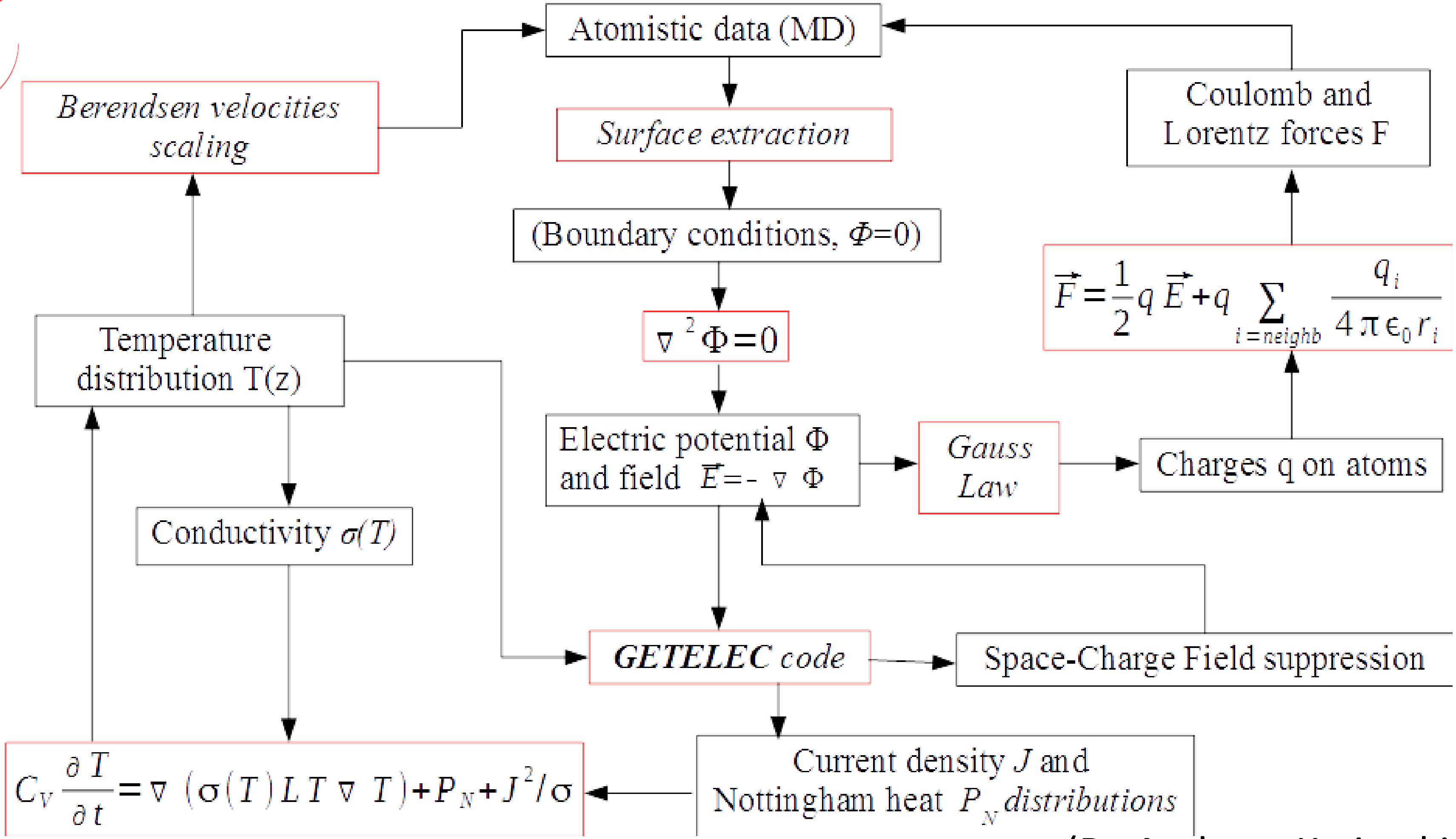
- *What is the mechanism leading from intense field electron emission to plasma formation?*

The way to answer is to include many phenomena in MD simulations:

- Atomic movement and deformations – PARCAS (MD)
- Field distribution calculation on a flexible mesh – FEMOCS (FEM)
- Electron emission from sharp tips – GETELEC
- Joule and Nottingham heating - HELMOD
- Field-induced stress - HELMOD

(By Andreas Kyritsakis)

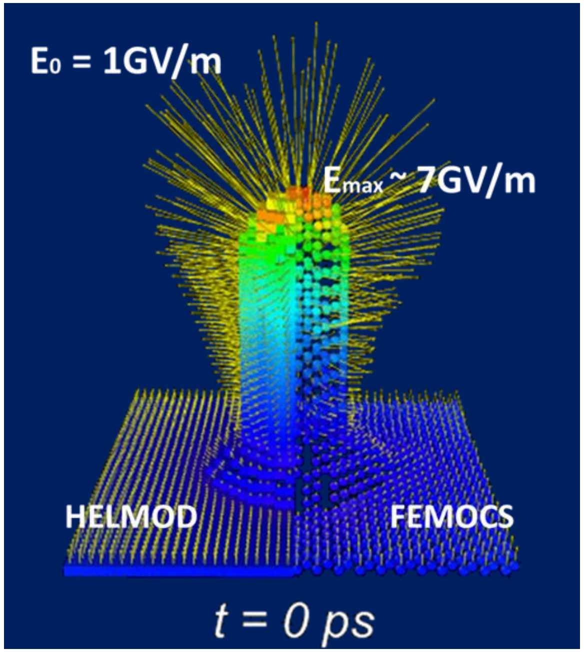
Integrated Multi-physics simulations



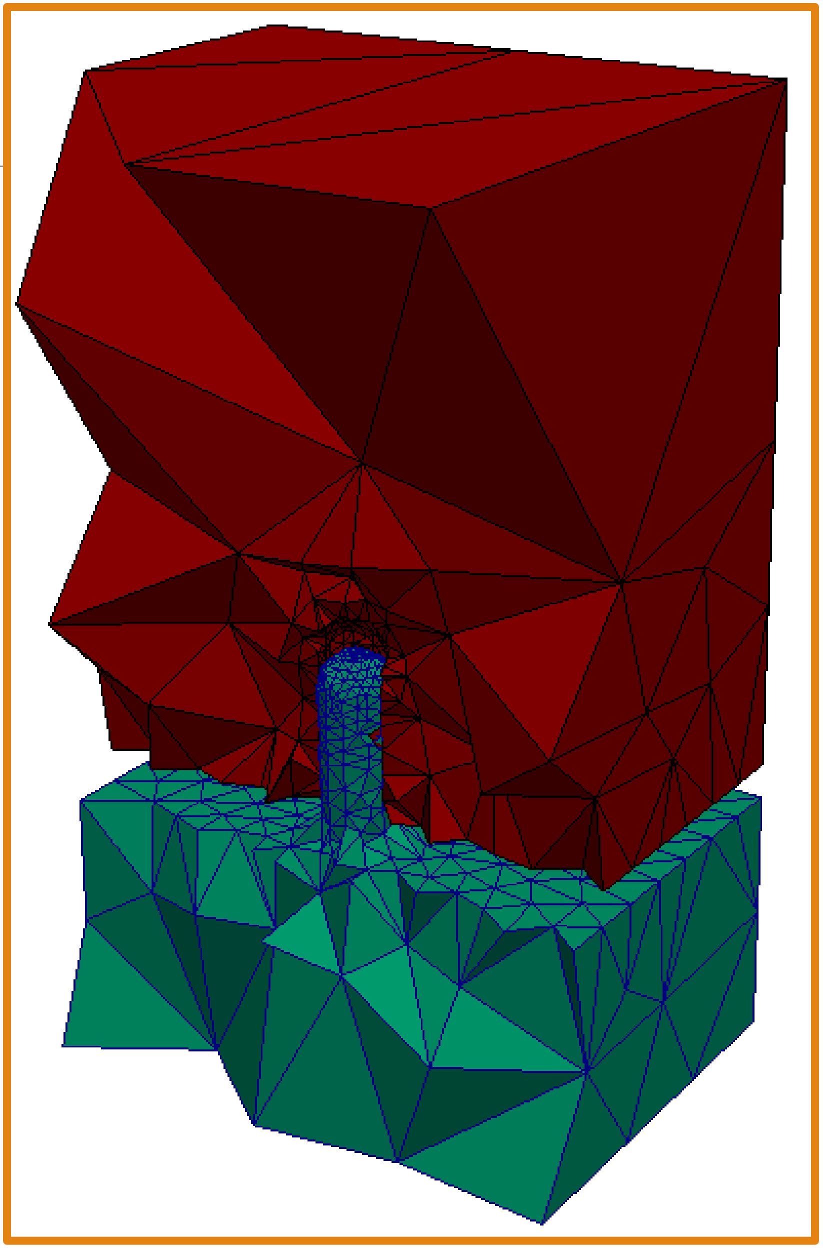
(By Andreas Kyritsakis)

Illustration of the elements in FEM

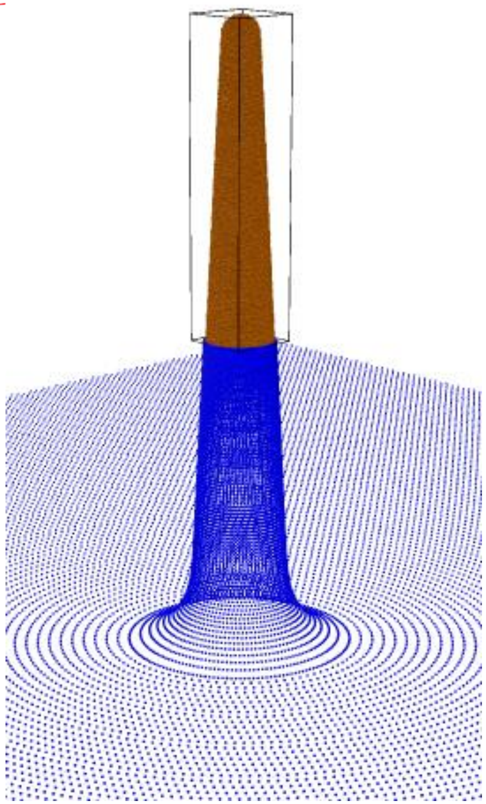
We now have an improved implementation of electric field in MD by using FEM elements. The calculations are more flexible and can reach large scales.



(By Mihkel Veske)



Simulation results: high tips



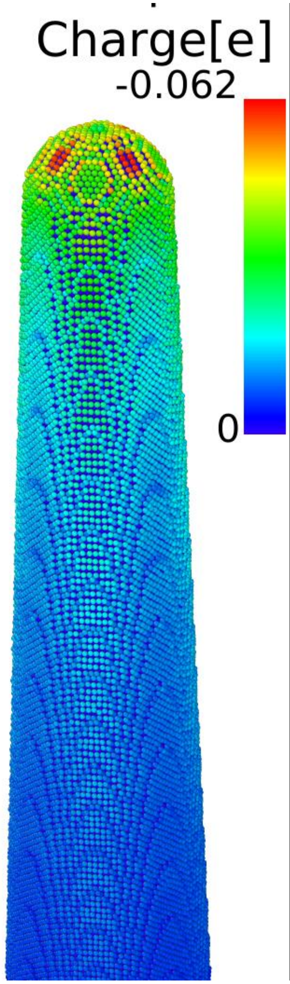
Experiments have shown enhancement factors of the order of β~20-50

Generate a tip with geometric aspect ratio (enhancement factor) of β ~30: h=92nm, R=3nm

MD – practically infeasible! To keep the CPU time within reasonable amount, we simulate only the interesting (upper) part of the tip with MD.

The bottom is extended surface in order to calculate correctly the field with the FEM

Impoved model of Helmod



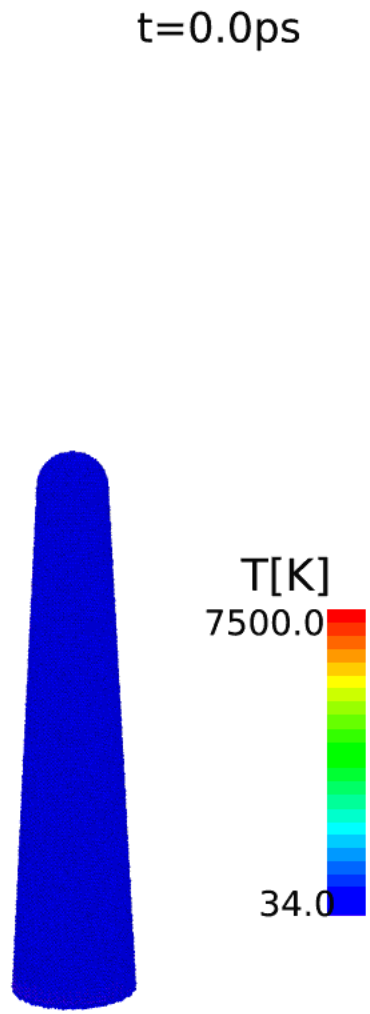
Surface charge due to applied field is distributed to the discrete atoms

A Lorentz force is induced to that charge

Interesting observation:

- Atoms in a close-packed facets receive less charge per atom

Finally – Thermal runaway: nanocluster evaporation



The emission current cause Joule and Nottingham heating

The high temperature:

Increases the thermal and electric resistivity

Makes the tip “flexible” and the top atoms more mobile

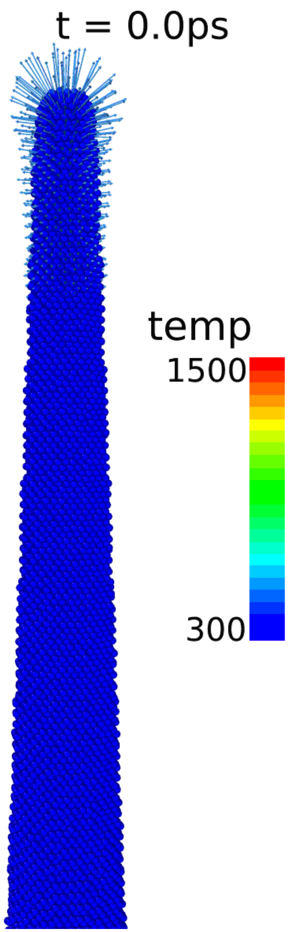
The field-induced stress deforms the apex and pulls the mobile atoms making it pointier

The field and hence the emission current are locally enhanced

More heating. Positive feedback. Thermal runaway!!

Evaporation of large parts of the tip in forms of atoms and nanoclusters

Size effect: the same β, but 3 times smaller

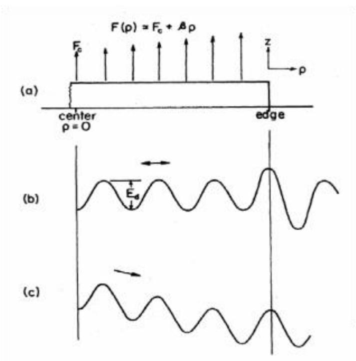


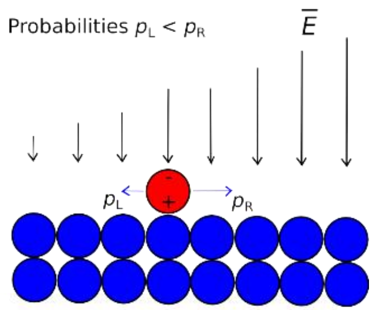
If the tip is smaller, the surface minimization stress is more intensive than the field-induced stress

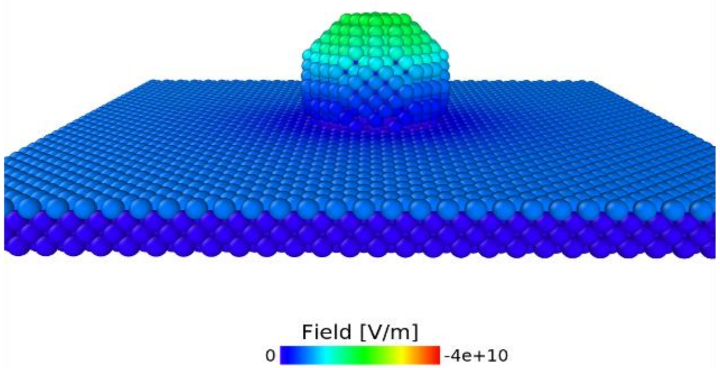
Although the tip initially heats to melting point it swiftly collapses

The height goes down and the field-induced forces are reduced significantly

Long term surface – electric field interaction







Adatoms in electric fields become polarized

This introduces a dipole force, 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

The bias of the adatom migration is achieved by using migration barriers modified by the field at the lattice point (0) and the saddle point (s):

$$E_m = E - (\mu_s F_s - \mu_0 F_0) - \frac{1}{2}(\alpha_s F_s^2 - \alpha_0 F_0^2)$$

μ_0 and α_0 = αs are calculated with DFT

μ_s is fitted to experiment

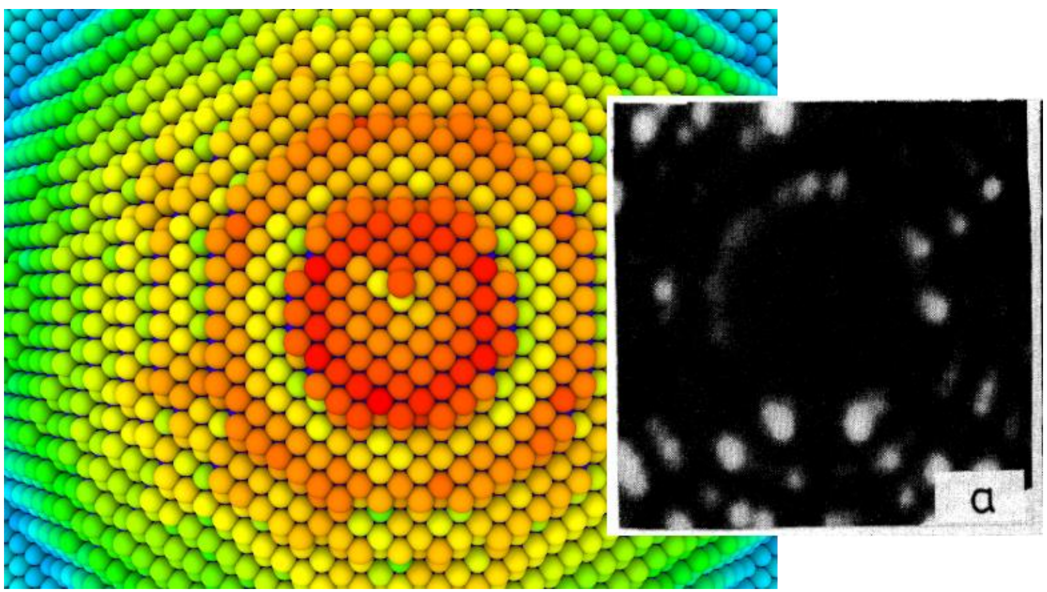
[Tsong & Kellogg PRB 1975]

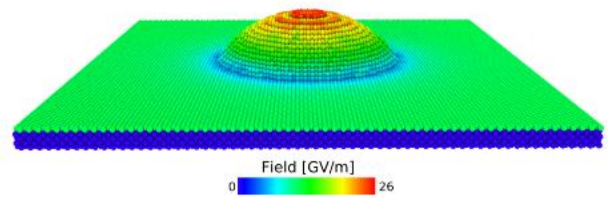
Ville Jansson

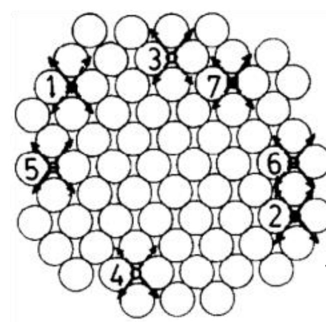
Reproducing experiments

Experiments [Wang & Tsong PRB 1982] were performed on the top of a W tip (W{110}) . Imaging was done by FIM, the possible ending positions were identified

We can compare the drift velocity of a single W atom on surface in a field gradient with experiments



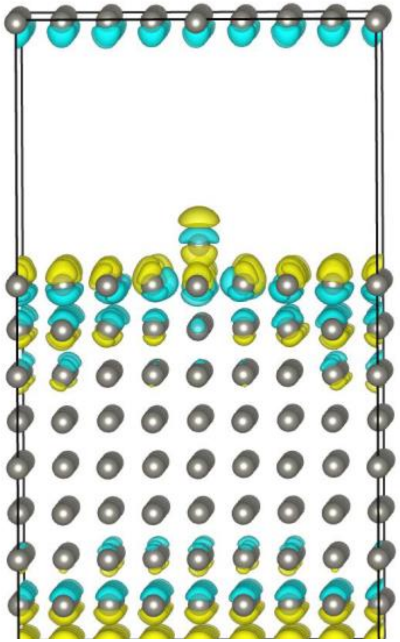




Ville Jansson

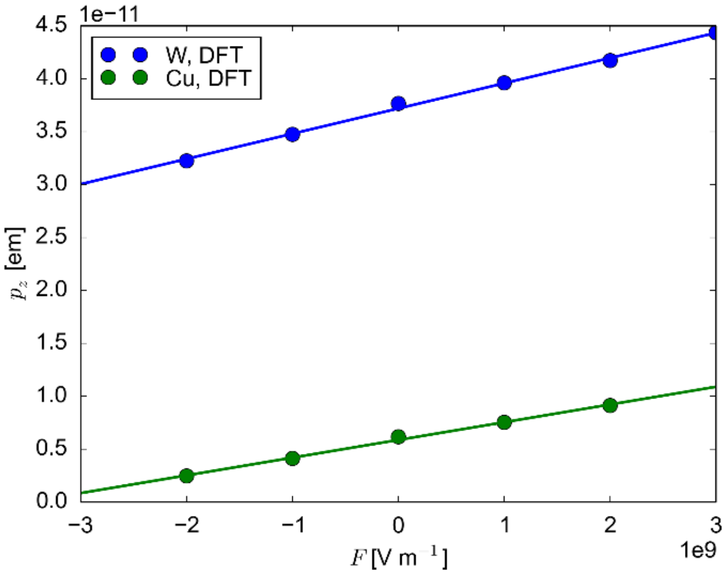
DFT calculations : atomic diffusion under electric field

Charge distribution under high electric field obtained as a difference between the DFT simulations with no field and simulations under 1 GV/m field. Yellow color corresponds to the accumulation of electrons, blue - depletion. Electric field direction is into the slab, i.e. direction of the force on electrons is from the slab to the vacuum



Dipole moment and polarizability of W and Cu adatoms were calculated with VASP

In the figure to the right is the force acting on electrons in eV/A vs dipole moment calculated with VASP for W adatom on W. The slope of the fitted line is the polarizability of an adatom

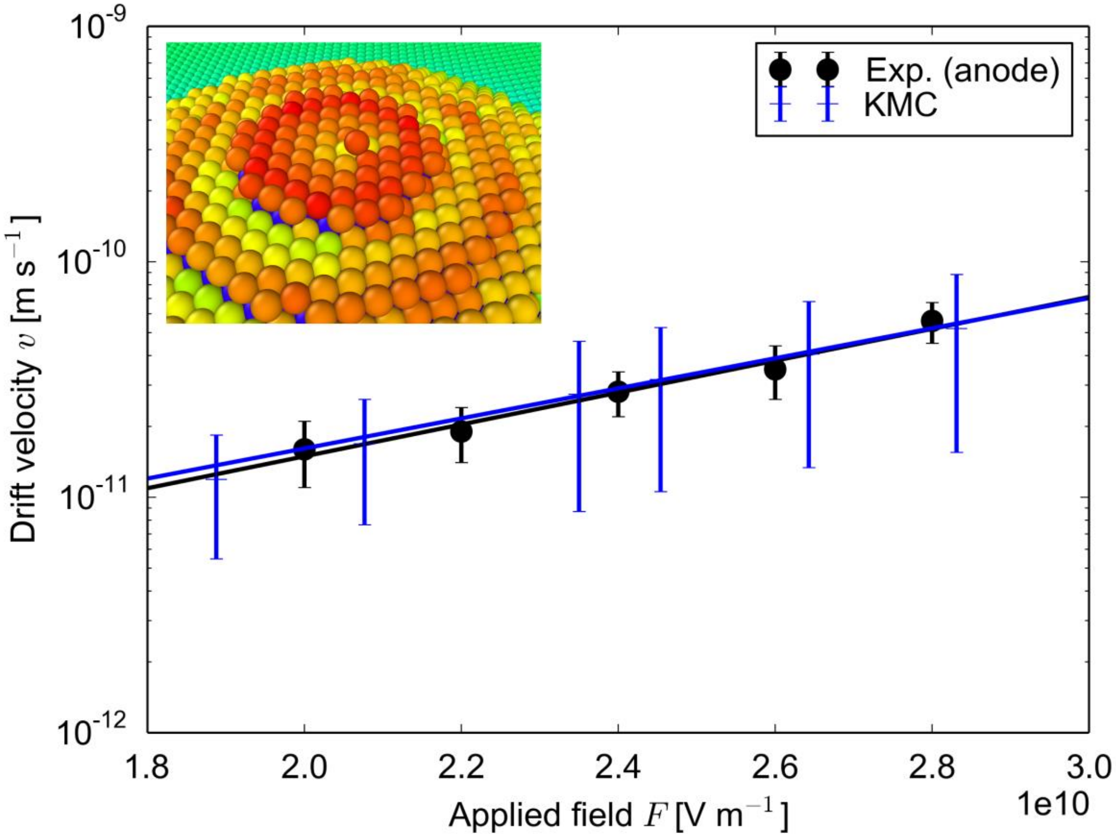


Ekaterina Baibuz)

Surface diffusion in electric fields

Comparison with experiment

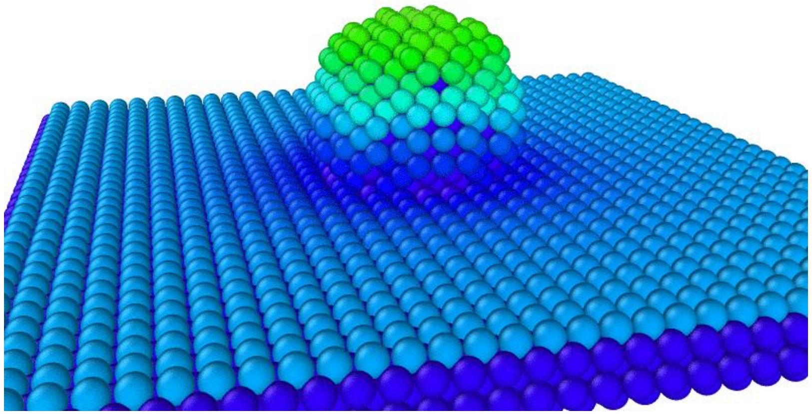
We get excellent agreement between our model and experiment

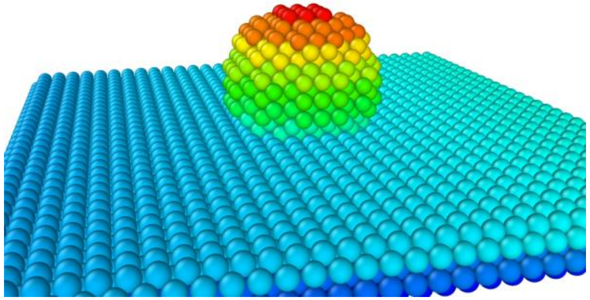


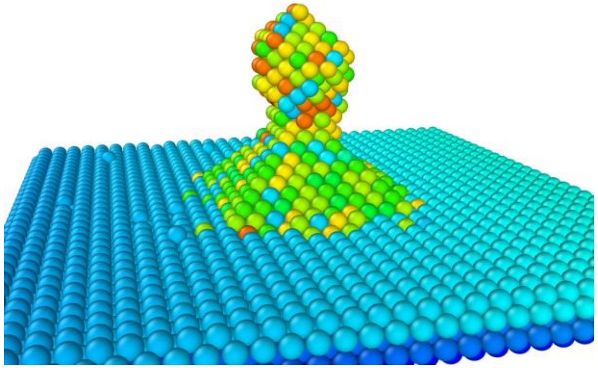
Ville Jansson

Surface diffusion in electric fields
Growth of W nanotips

Colours according to the initial atom positions to show the diffusion



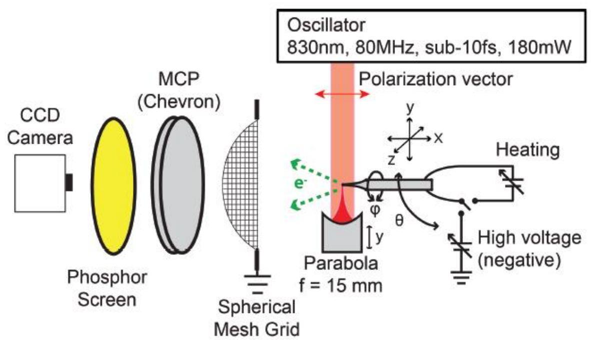


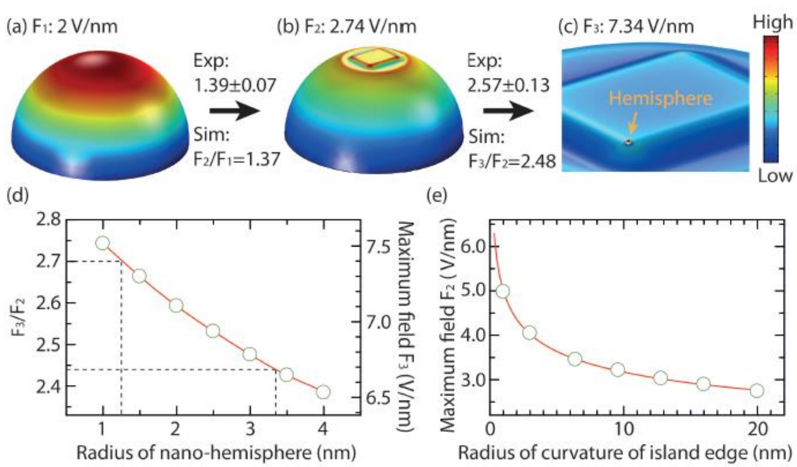


W nanotip at 3000 K in 1 GV/m applied field (atoms are colored according to the field)
The bias diffusion in fields causes formation of nanotips

Ville Jansson

Static surface under electric field and fs-laser irradiation



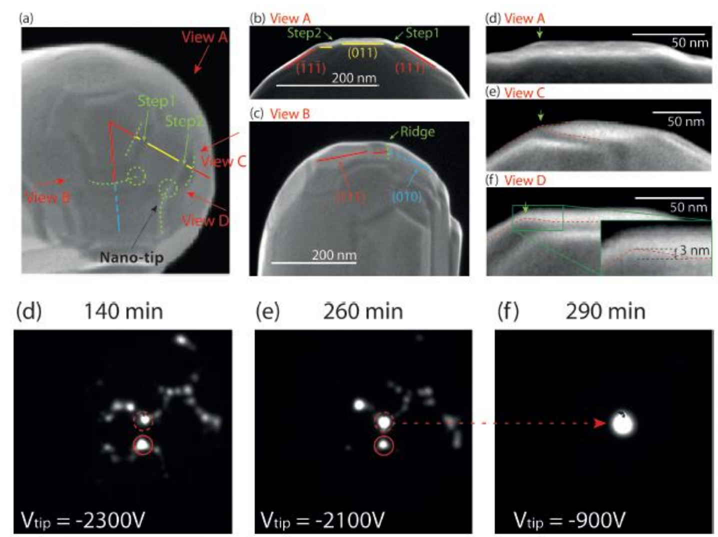


Field Emission Microscopy experiment

Collaboration with Dr. Hirofumi Yanagisawa(Max-Planck Institute of Quantum Optics)

Surface faceting and protrusion formation

Possible mechanism for emitter formation



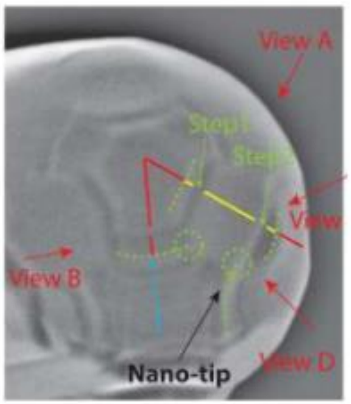
H. Yanagisawa, V. Zadin et al., APL Photonics 1 (2016) 091305

Vahur Zadin

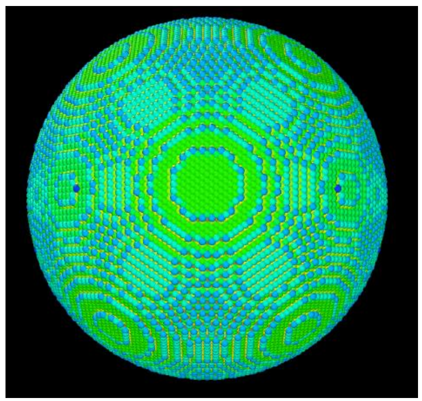
Laser-induced heating and faceting on a tungsten tip

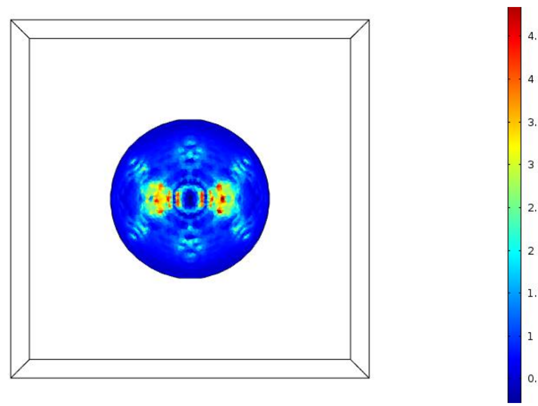
Field electron emission, including work function effects

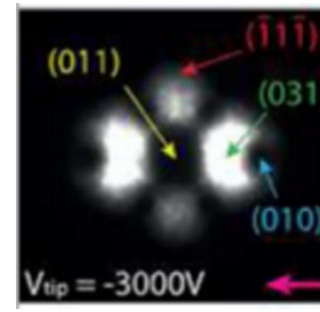
Excellent agreement with experiments

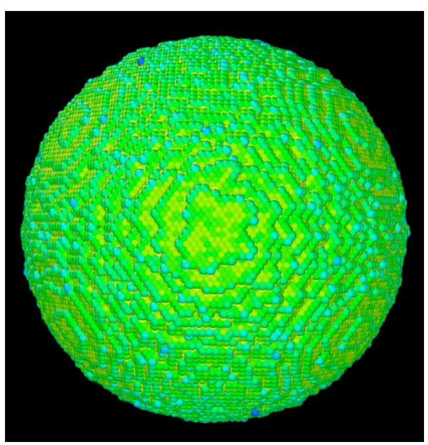


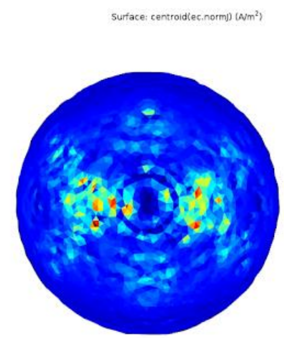
https://arxiv.org/pdf/1605.05393.pdf

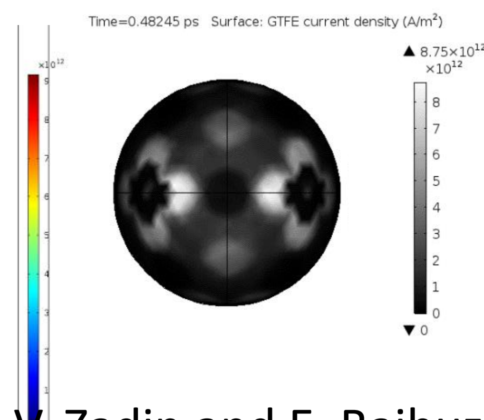






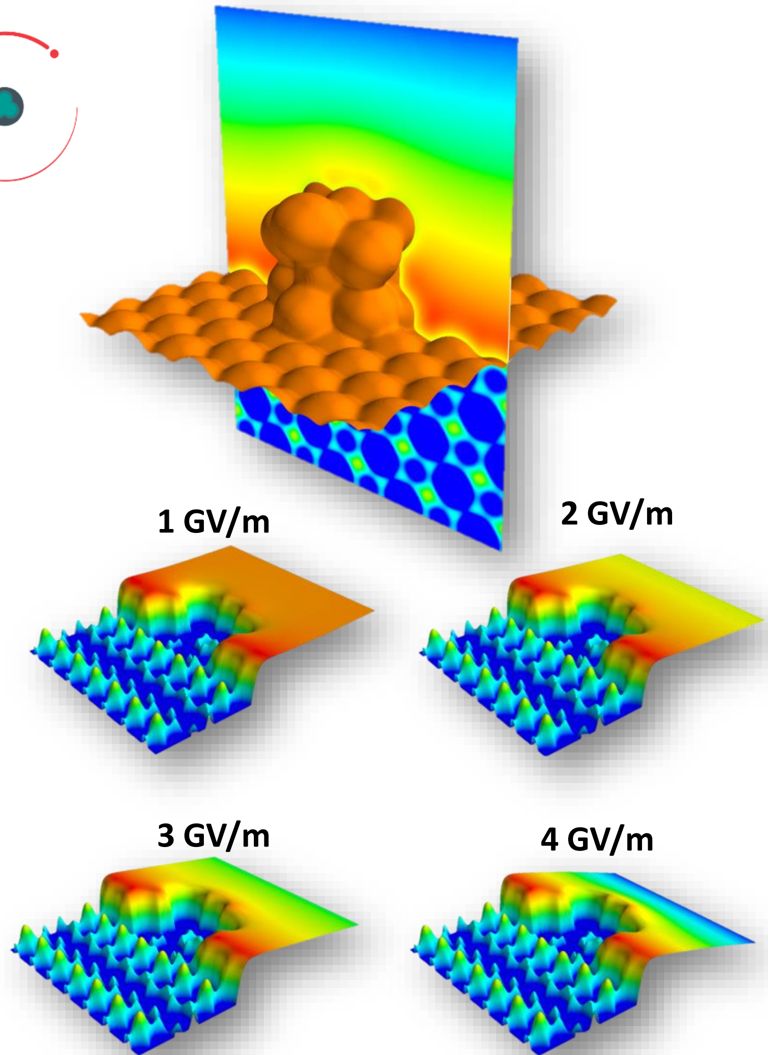






V. Zadin and E. Baibuz

Potential landscape around defects



Potential landscape for different rough surface features with DFT under electric field

DFT calculations done for multiple electric field values (potential shown for a geometric slice)

Complex potential landscape is formed due to the surface protrusions

Application of Schottky-Nordheim barrier for such defects questionable

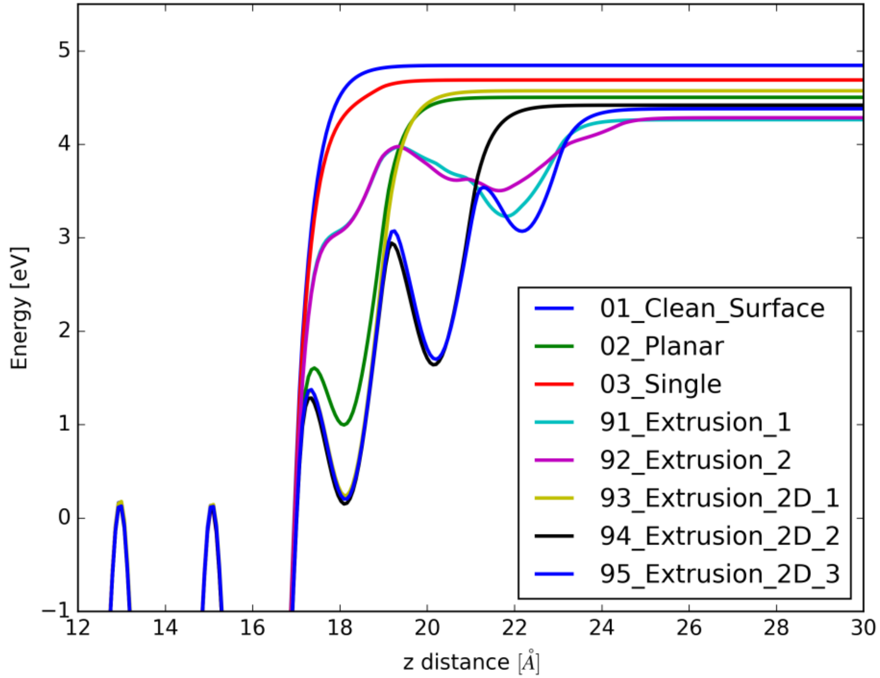
Difficulties with surface curvature corrected barriers expected as well (GETELEC code)

Possible solution for work function estimation based on estimation of electron tunneling probabilities

Kristjan Eimre

Work function decrease due to surface defects

Geometry	WF (eV)	dWF	%
Extrusion 1	**4.26**	**0.58**	**12.0%**
Extrusion 2	4.28	0.56	11.6%
Extrusion 2D 3	4.38	0.46	9.5%
Extrusion 2D 2	4.42	0.42	8.7%
Planar	4.50	0.34	7.0%
Extrusion 2D 1	4.57	0.27	5.6%
Single	4.69	0.15	3.1%
Clean Surface	**4.84**	**0.00**	**0.0%**



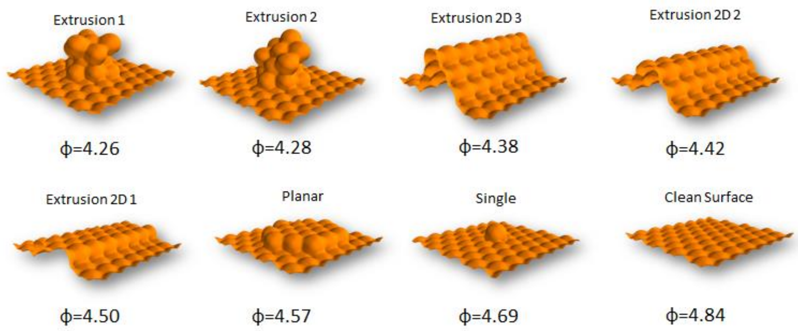
Smooth 111 surface from literature:

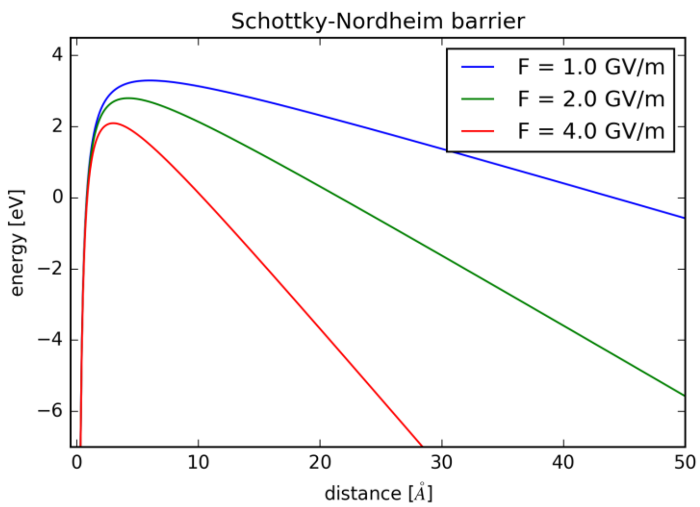
4.85 (Gartland, P. O., Slagsvold, B. J.: Phys. Rev. B 12 (1975) 4047)

4.88 (Kubiak, G. D.: Surf. Sci. 201 (1988) L475.)

Changes in work function due to electric field

Geometry	No field	1 GV/m	2 GV/m	4 GV/m
Clean surface	**4.84**	**4.84**	**4.84**	**4.84**
Planar	4.50	4.63	4.45	4.38
Single	4.69	4.78	4.65	4.61
Extrusion 1	4.26	4.26	3.96	3.83
Extrusion 2	4.28	4.22	3.88	3.53
Extrusion 2D 1	4.57	4.64	4.49	4.44
Extrusion 2D 2	4.42	4.43	4.24	4.14
Extrusion 2D 3	4.38	4.35	4.12	3.93





Quantum transportation calculations to evaluate change in work function and barrier height

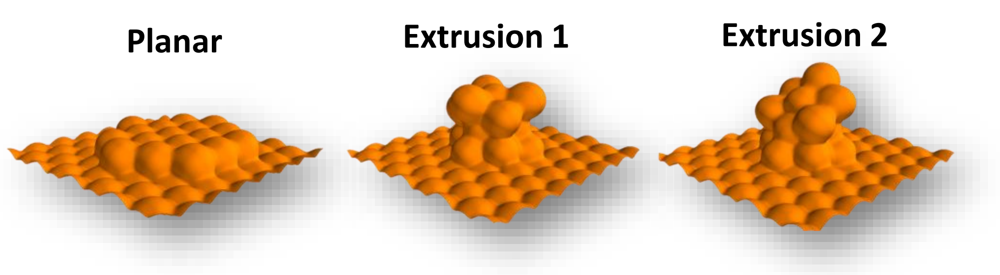
Dependence on geometry and external field

System energies

- General trend – system energy decreases when electric field is applied
- Field makes surface modifications more stable
- Surface with islands preferred over surface with adatoms
- Good agreement with previous KMC simulations by V. Jansson
- Effect observed in experiments as well
- Applied field lowers planar defect energy below the flat surface energy
- Surface roughening due to field energetically favorable

Energy per atom for all geometries (in meV = 10^{-3} eV)

Field (GV/m)/ Geometry	0	1	2	4
Clean Surface	**0.0**	**-0.36**	**-1.45**	-5.81
Planar	**3.67**	3.46	2.50	**-1.69**
Single	**3.90**	3.61	-	-
Extrusion 1	**24.85**	**24.72**	**23.71**	**13.93**
Extrusion 2	**24.62**	**24.46**	**23.42**	**-**
Extrusion 2D 1	0.70	0.46	-	-
Extrusion 2D 2	5.94	5.72	-	-
Extrusion 2D 3	12.78	12.56	-	-



Summary

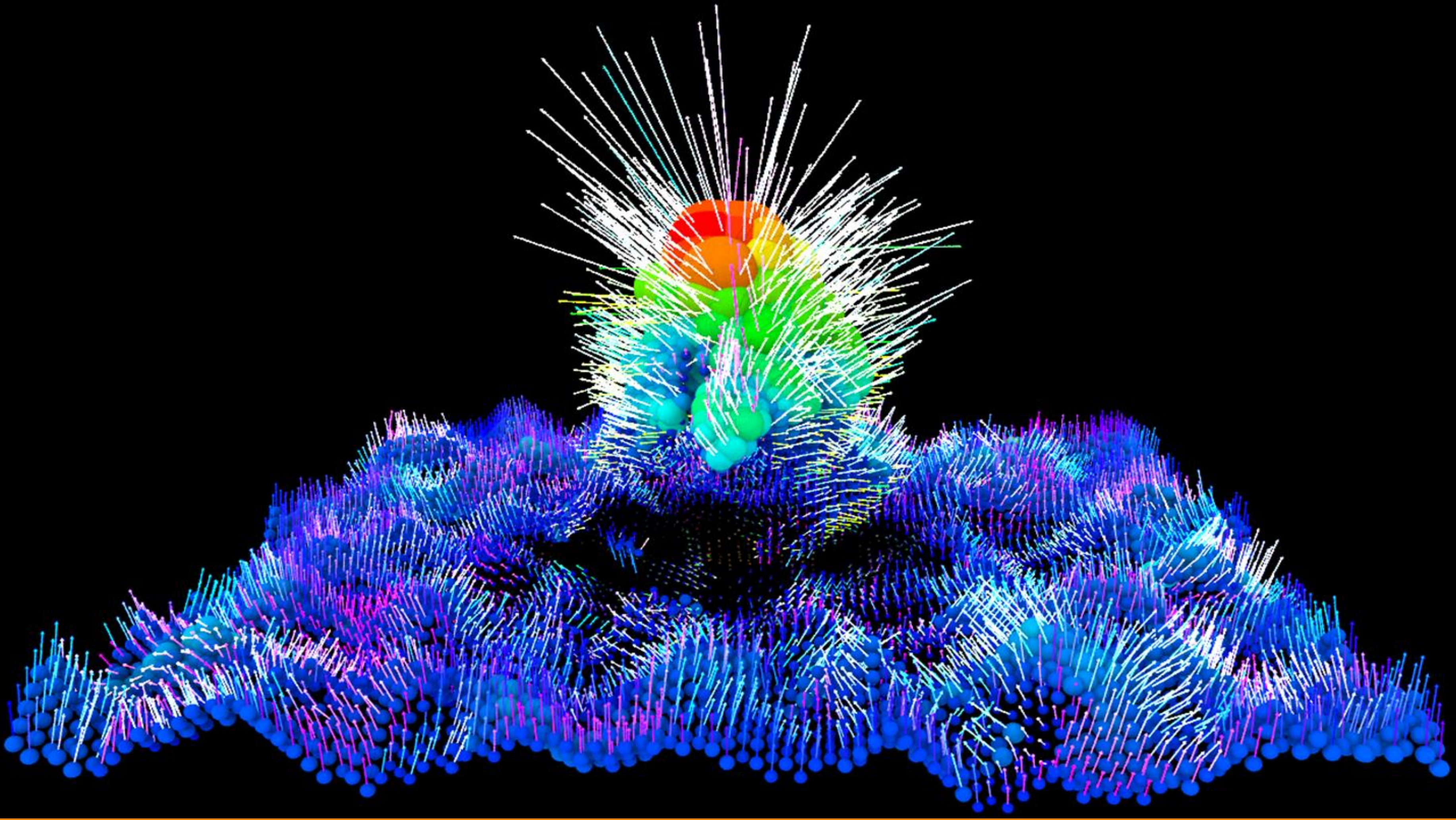
We are starting a new page in our research.

We start in-house experiments in collaboration with the DC breakdown group at CERN

We have the electric effects in our atomistic models, both molecular dynamics and kinetic Monte Carlo

Kinetic Monte Carlo shows that at high fields indeed a growth is possible due to surface polarization effects

More accurate calculations by using DFT methods show a significant decrease of the workfunction near rough surface features.



Thank you for your attention!