Multiscale simulation Model of Electrical Breakdown: current status and perspectives

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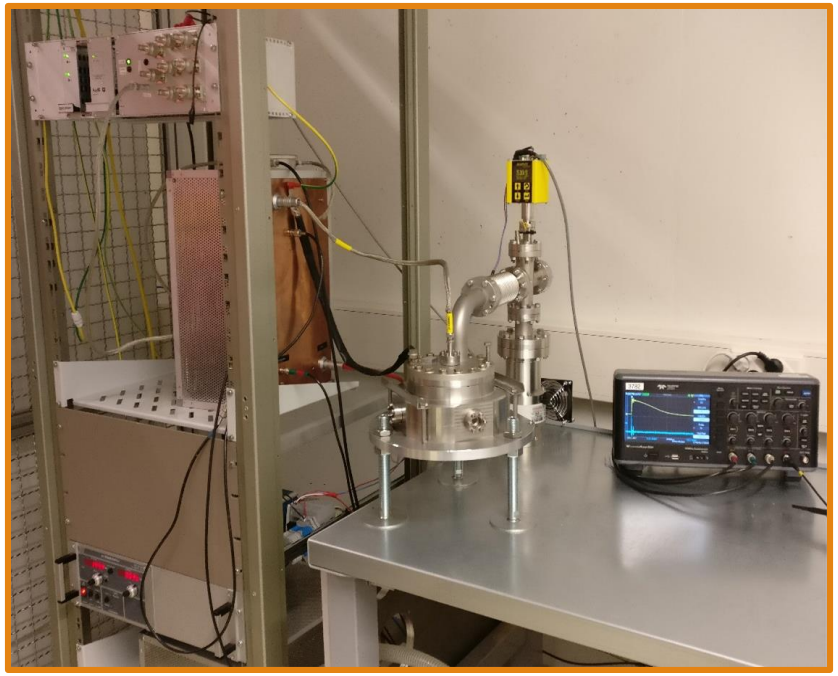
A new home for LES @ Helsinki: Current status by A. Saressalo

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



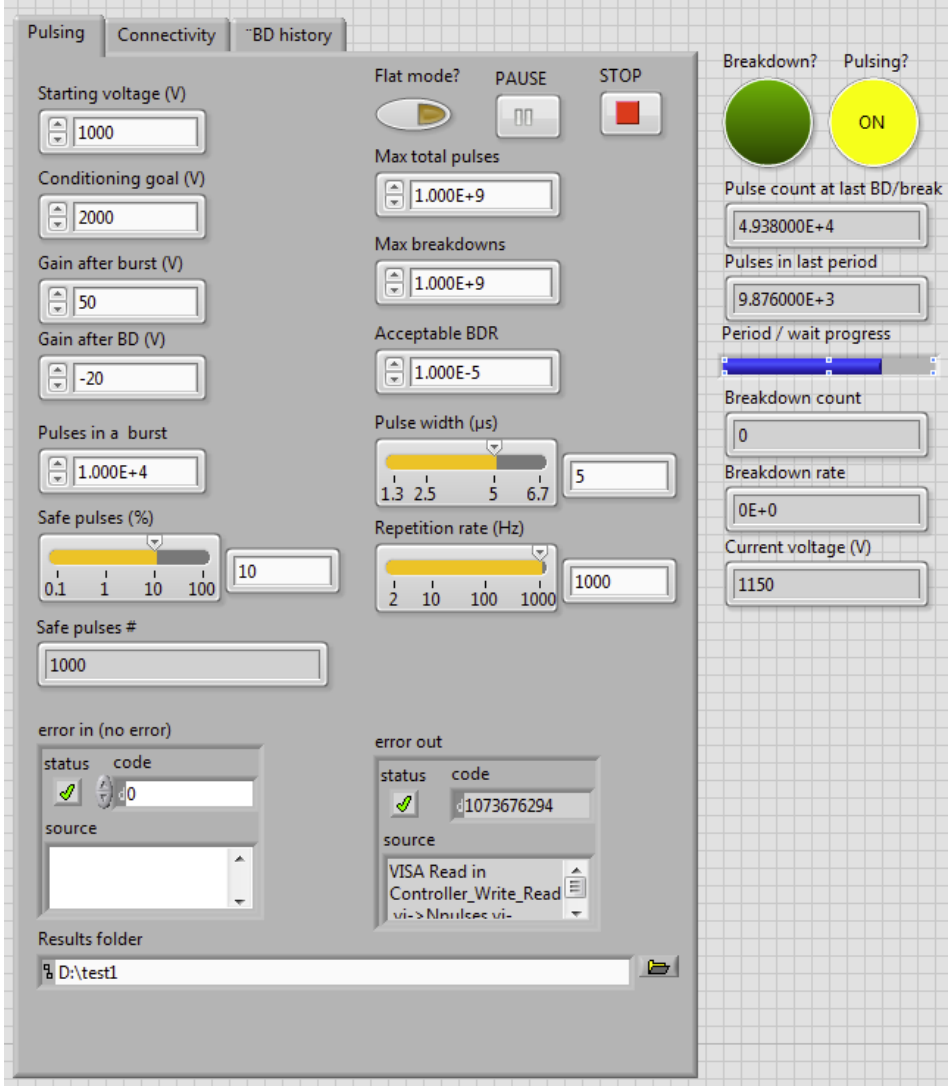
Current challenges and outlook

Unfortunately, there are still some challenges:

- Controller stops responding to commands without any apparent reason
- Controller cool-down time after a BD varies between 5 - 100 s
- Longer runs currently are not possible without manual interaction

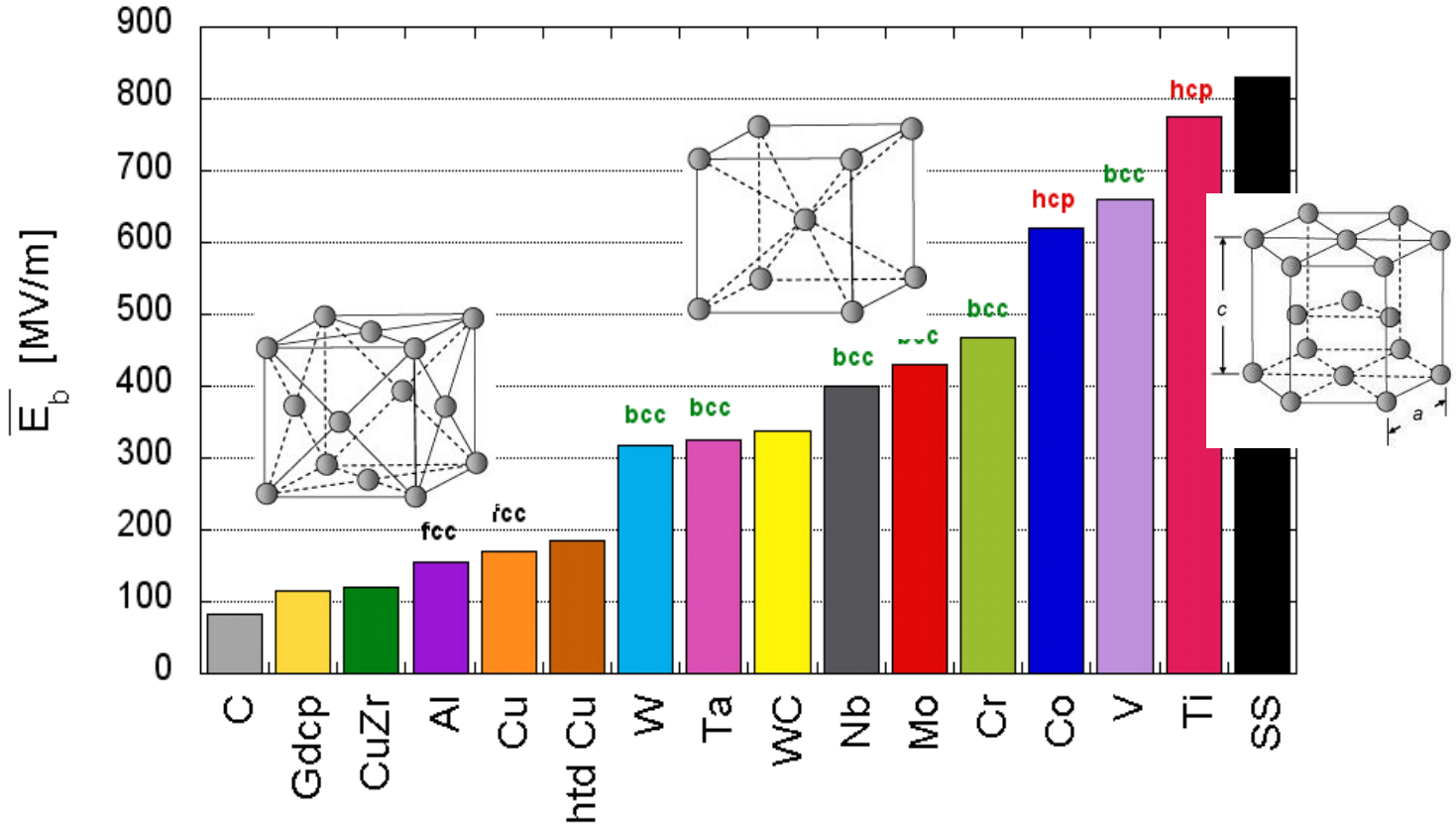
What we plan to do:

- Improve the program to catch the unexpected behavior
- Also use an oscilloscope to confirm the breakdowns
- Automatize statistical calculation and
  necessary plotting



Our search for dislocation-mediated mechanisms

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.

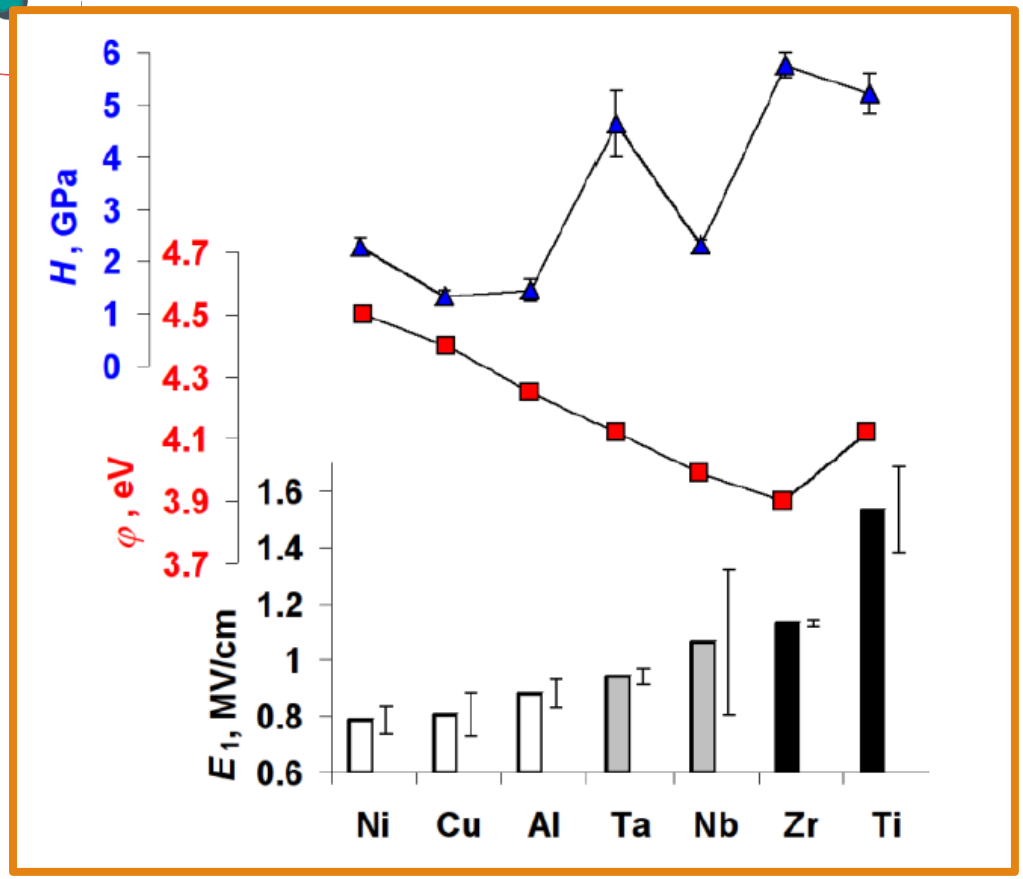


A. Descoeudres, F. Djurabekova, and K. Nordlund, DC Breakdown experiments with cobalt electrodes, CLIC-Note XXX, 1 (2010).

Independent study in Tomsk, Russia

Different experiment, different surface treatment, different condition.

The trend is… the same!



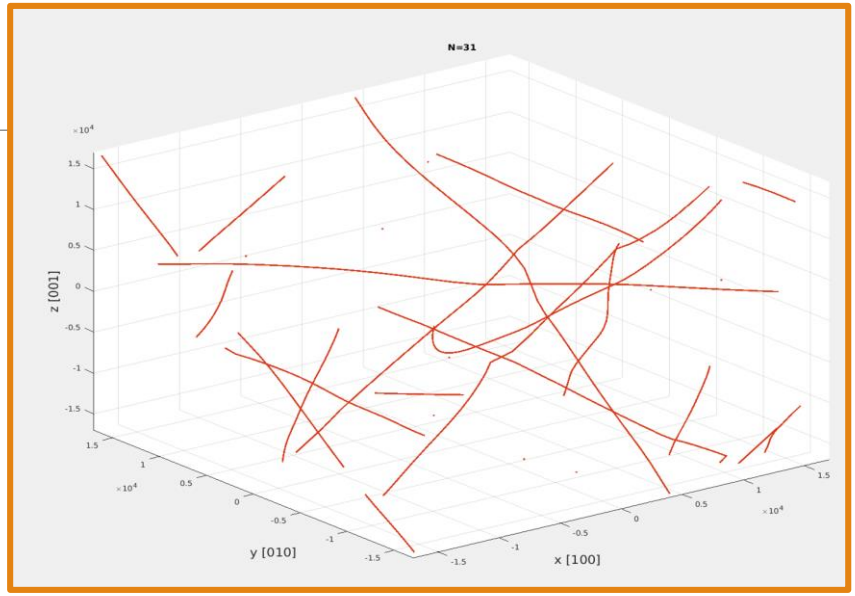
Microhardness, electron work function (values recommended in [24]), SPES *E*1, and crystalline structure (empty bars – FCC, half-tone bars – BCC, solid bars – HCP) vs the electrode pair materials

[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]

Dislocation dynamics: DDD simulations (A. Saressalo)

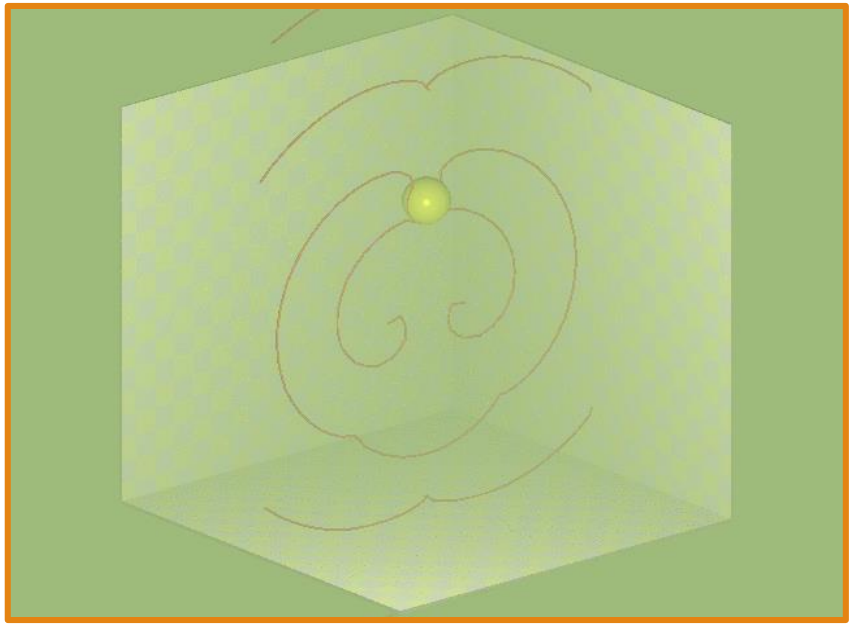
ParaDIS code:

- Parallelizable 3D dislocation dynamics
- Built-in dislocation interactions
- Mobility functions for FCC and BCC metals



Under construction:

- Dislocation interactions with precipitates
- Afterwards implementation of other obstacle types



FEMOCS by M. Veske

In our group we have developed a concurrent molecular dynamic electrodynamic model to simulate the effect of electric field dynamically. However, it has proven to be not sufficiently flexible at high temperatures:

- many atoms move fairly far away from their original positions, too far from rigid lattice.
- The rigidness of the model was dictated by rigid grid of finite difference method to calculate the field

FEMOCS is a new code to deal with large and dynamic atomic systems

It uses the finite element method (FEM), which enables the larger systems of atoms

- two orders of magnitude more atoms than previously

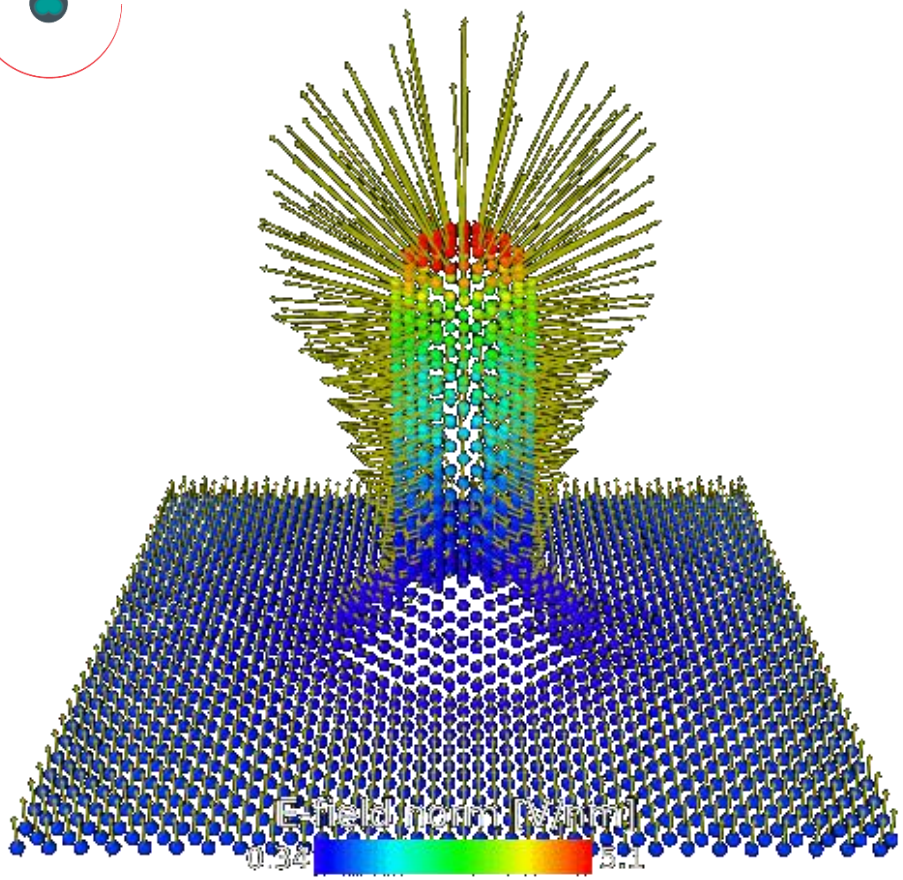
Any crystal structure and orientation, including amorphous systems

Low cost of extending the empty space – less atoms in MD / kMC

(partial) support for parallel computations

Illustration of distribution of electric field and force on surface atoms by FEMOCS

Electric field



Electrostatic force

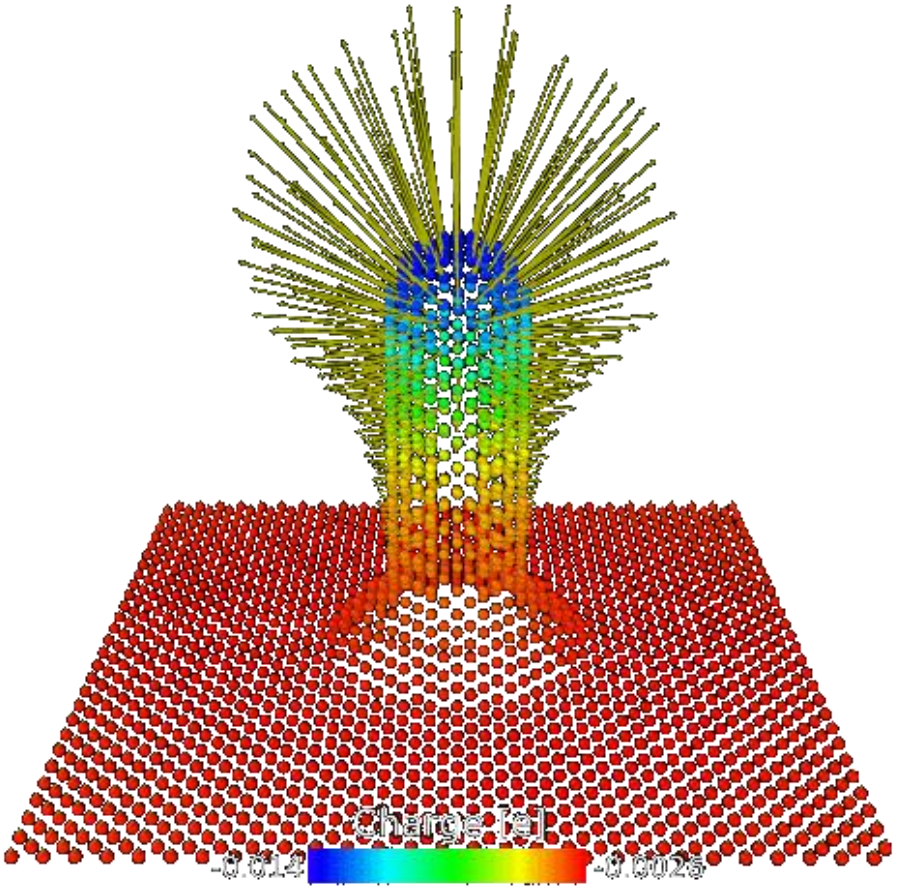
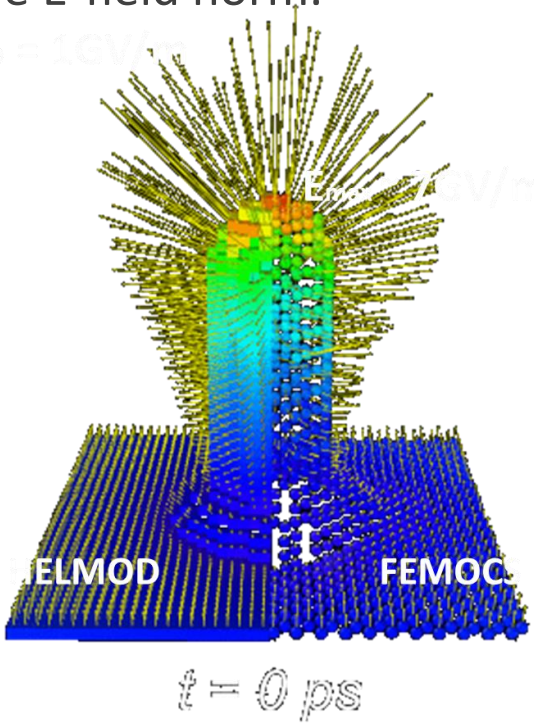
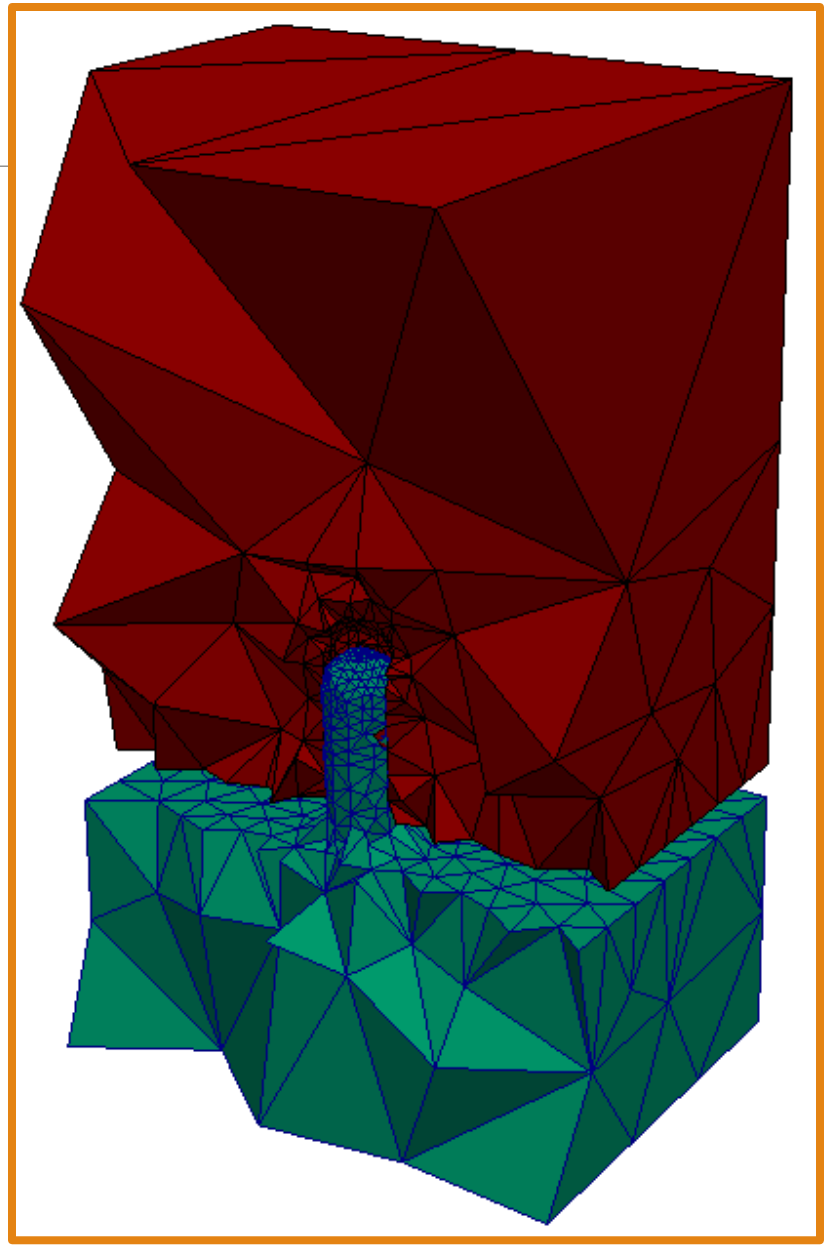


Illustration of the elements in FEM. Verification.

Comparison of the current approach compared to the existing HELMOD model. In the figure coloring shows the E-field norm.



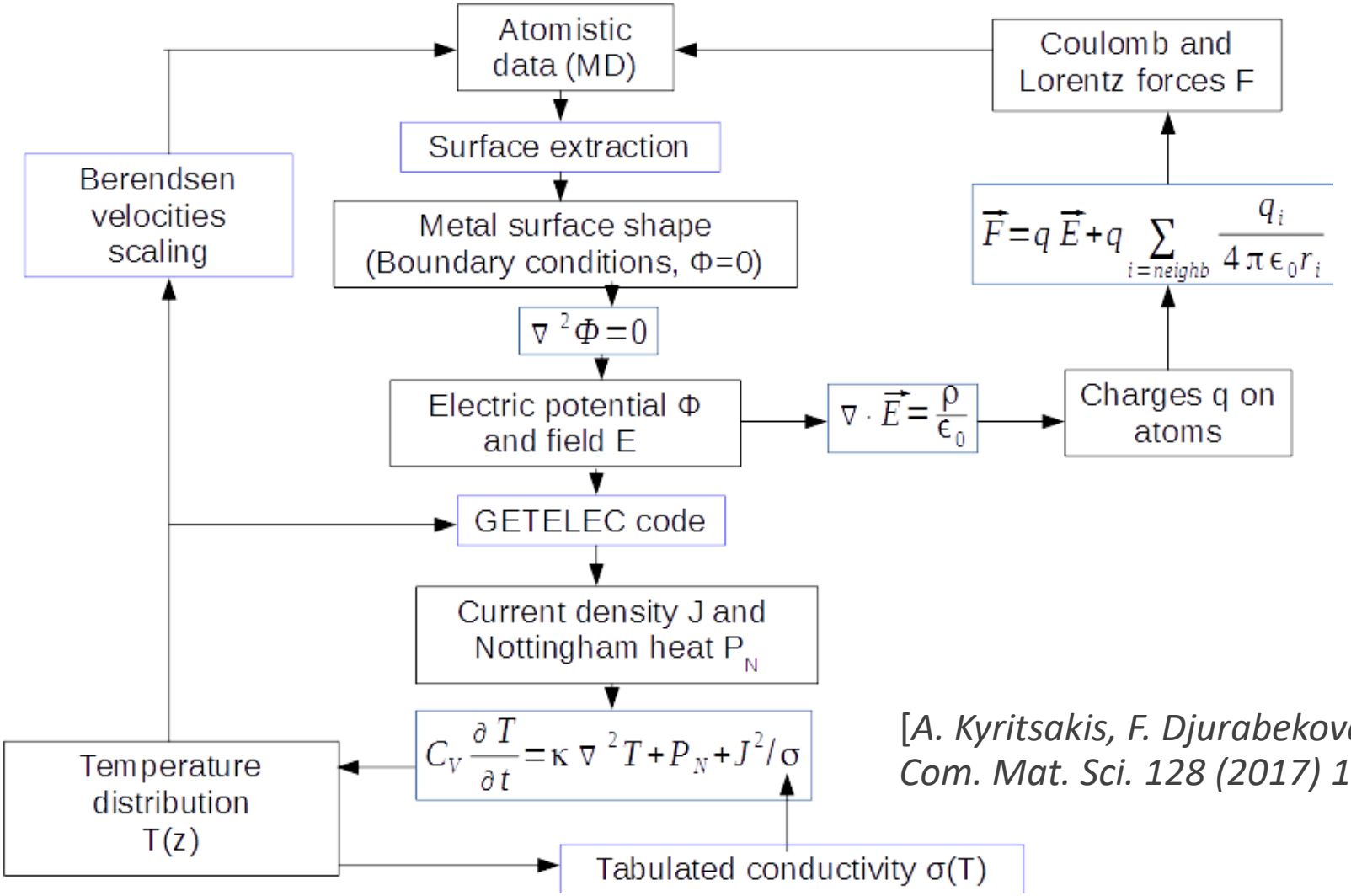


Electric field effects in MD simulations (A. Kyritsakis)

Effect of electric field on metal surface can be considered twofold:

- From the point of electronic dynamics
- Charge induced on metal surface will affect atomic evolution of the surface.
- Recently, a code GETELEC was developed by Andreas Kyritsakis [*A. Kyritsakis, F. Djurabekova, Computational Materials Science 128 (2017) 15–21*]. The code is able to account accurately and in efficient manner the field emission effects on atomic dynamics: Joule heating inside the tips and Nottingham effect at the very surface of the top of the tip. The heat generated by both processes is fed back to the molecular dynamic simulations.
- In collaboration with Mihkel Veske, a new more flexible approach to calculate the electric field around large structures on metal surfaces is developed and now available for MD simulations of relatively large tips heated up by field emission effects, concurrently with electric field calculations.

implementation with an atomistic model



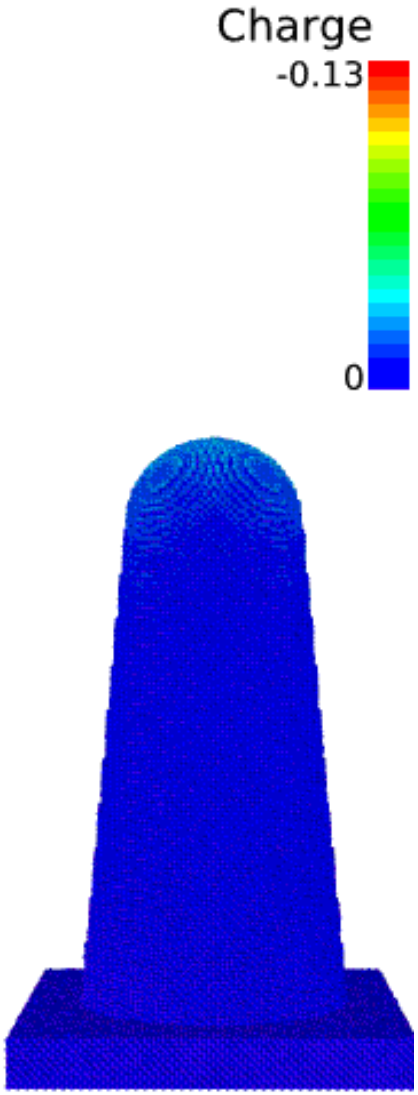
[*A. Kyritsakis, F. Djurabekova, Com. Mat. Sci. 128 (2017) 15–21*]

Evolution of a tip under high electric field
New FEMOCS

If the applied field is sufficiently high, it can melt the top of the tip. As a result, the tip enters in a positive feedback loop:

- The forces make it pointier and the current increases
- The current increases the temperature
- The temperature increases the thermal and electric resistivity and makes the tip more “flexible”

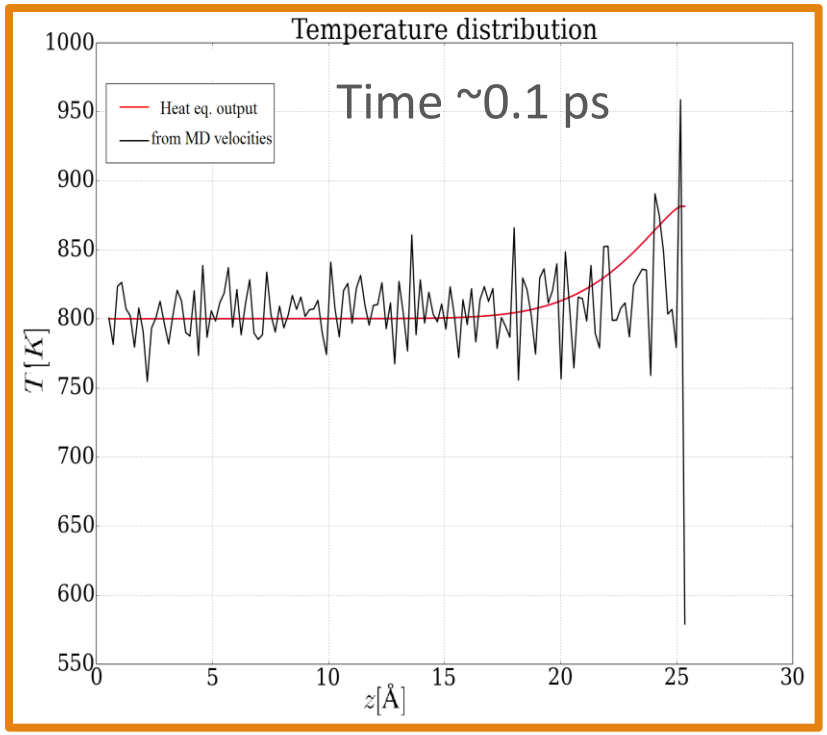
This will eventually lead to extremely high temperatures (might be exaggerated because we have neglected space charge effects) and evaporation of charged atom clusters

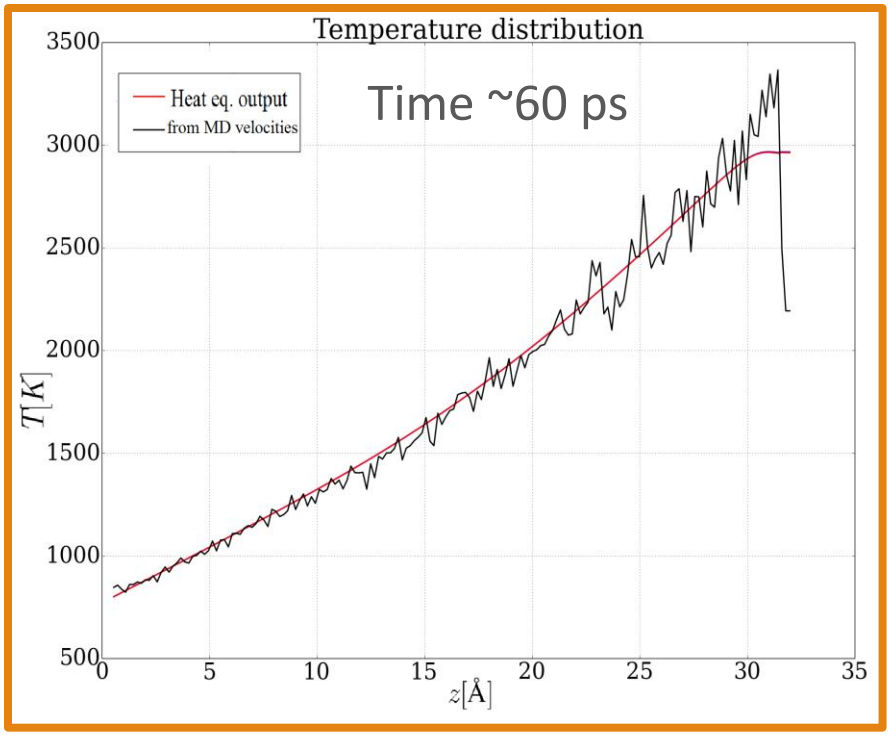


Temperature evolution in a tip

The positive feedback mechanism will eventually lead to extremely high temperatures (might be exaggerated because we have neglected space charge effects) and evaporation of charged atom clusters

The heat distribution starts growing due to mainly the Nottingham effect and finally reaches very high values





Surface diffusion in electric fields (V. Jansson)

Adatoms in electric fields become polarized.

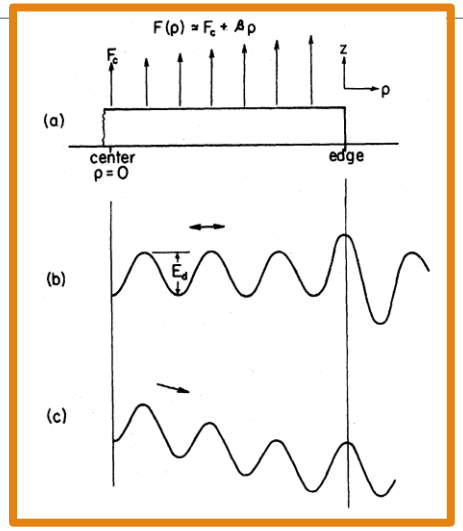
This introduces a dipole force, perpendicular to the field, that will bias the adatoms migration towards stronger fields

We have implemented this field effect into our Kinetic Monte Carlo (KMC) code Kimocs

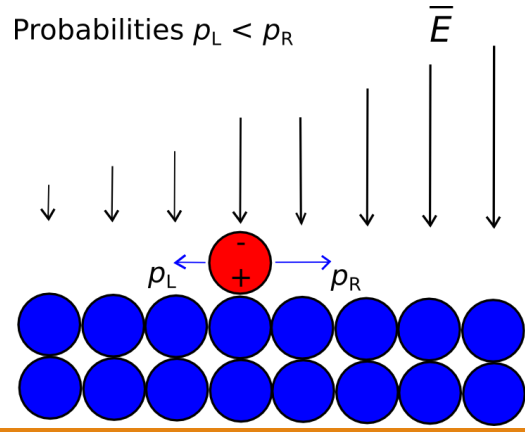
Directional walk is achieved by thermal activations and taking into account the reduction in potential energy.

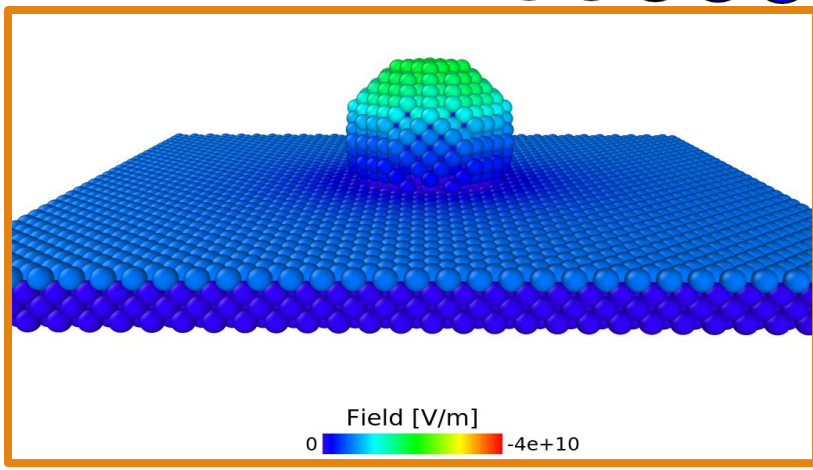
$$\Delta E(F) = E(0) - E(F) = \mu_t \Delta F + F_t \Delta\mu + \alpha_t F_t \Delta F + \tfrac{1}{2}(\Delta\alpha) F_t^2$$

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

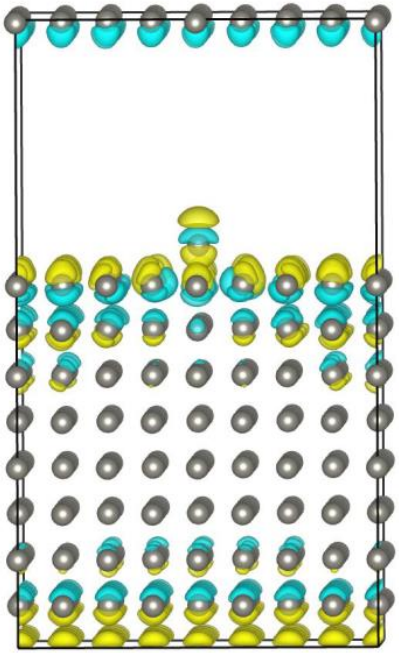


[Tsong & Kellogg PRB 1975]





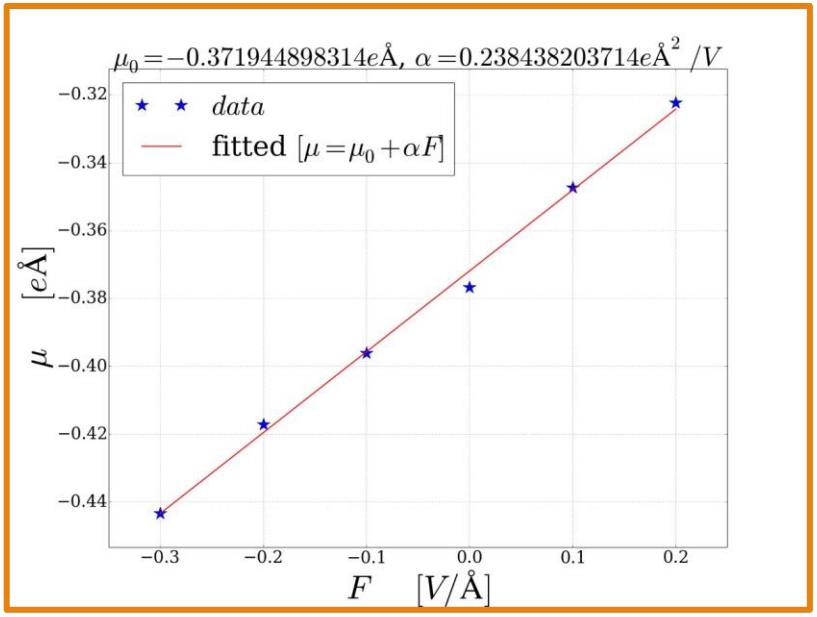
DFT calculations : atomic diffusion under electric field (E. Baibuz)



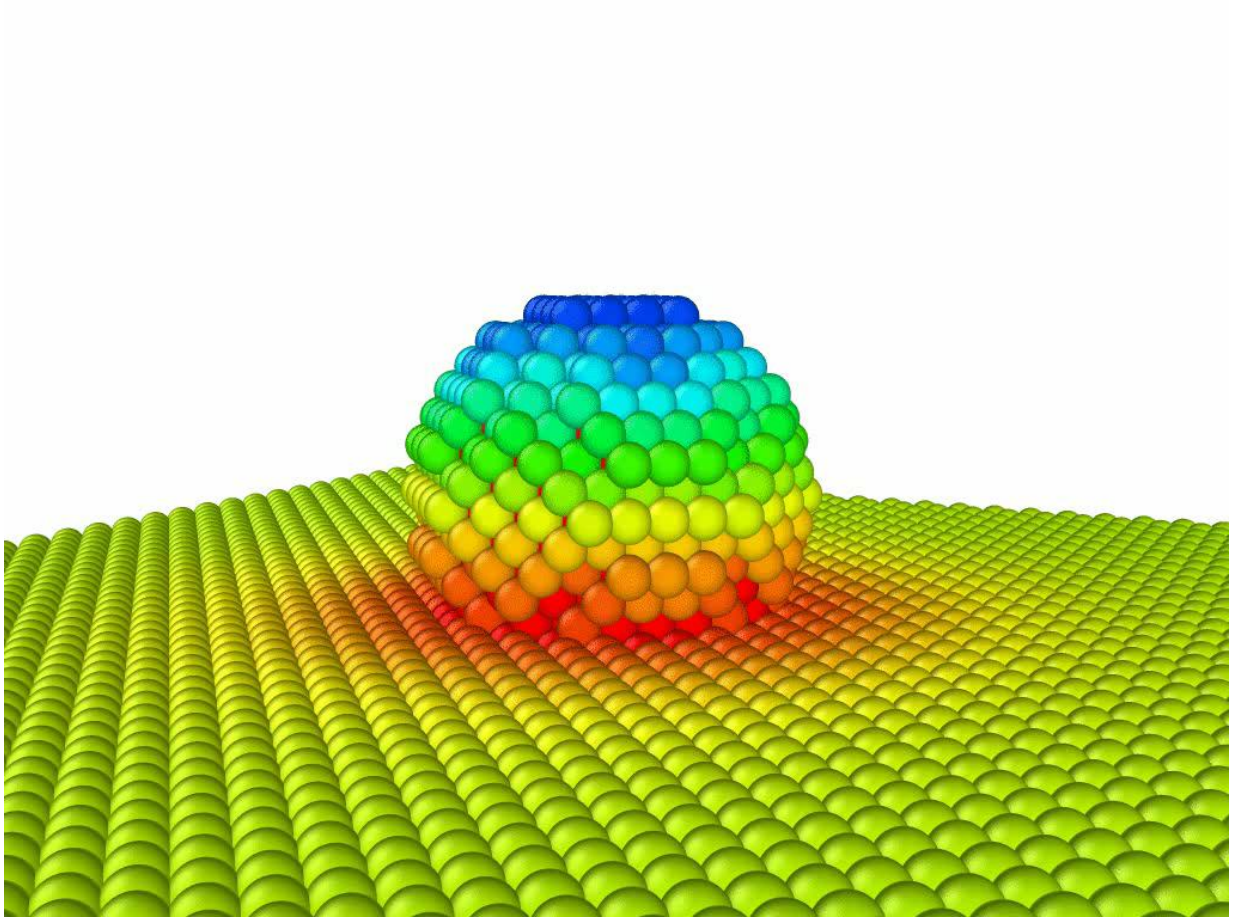
Charge distribution under high electric field obtained as a difference between the DFT simulations with no field and simulations under 1 GV/m field. Yellow color corresponds to the accumulation of electrons, blue - depletion. Electric field direction is into the slab, i.e. direction of the force on electrons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



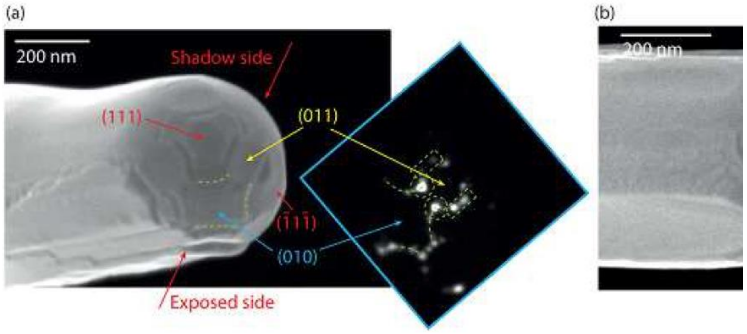
Evolution of a copper tip in the presence of high electric field

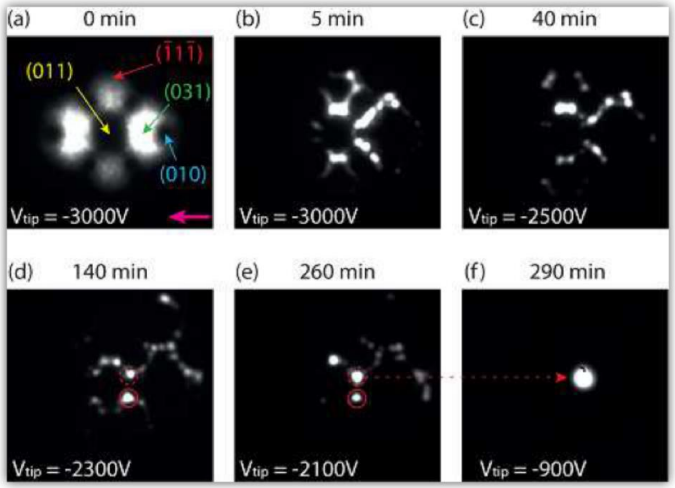


Nanotip growth on a tungsten tip under ultrafast laser + field emission

Experiment:

H. Yanagisawa, et al. APL Photonics (2016)





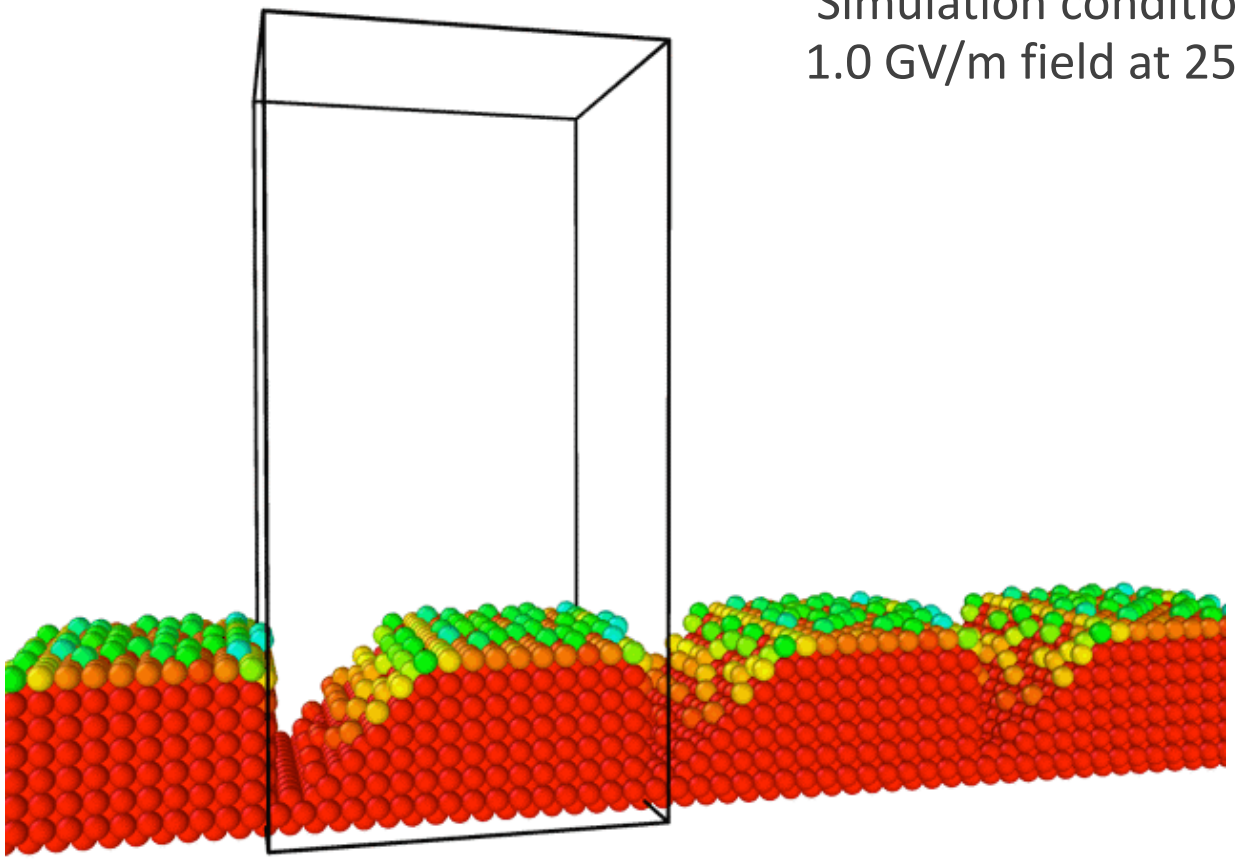
Simulations:

To address this problem we apply several different techniques:

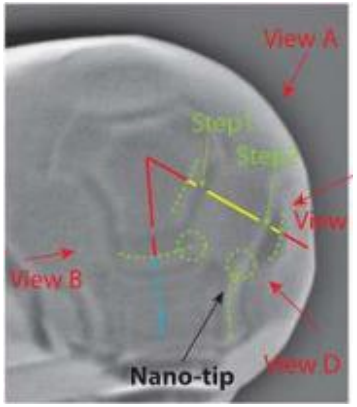
- The energy deposited to electron by a laser was calculated by H.Vázquez
- FEM to obtain stresses, lattice temperature etc. (Tartu)
- Molecular dynamics to analyze the formation of faceting under the possible temperature rise
- KMC to grow a tip on the surface

Growth of a nanotip on a W ridge by KMC by E. Baibuz

Simulation condition:
1.0 GV/m field at 2500 K



Asymmetric faceting effect on a laser-irradiated tungsten tip (V. Zadin)



Yanagisawa et al. APL Photonics 1 (2016) 91305

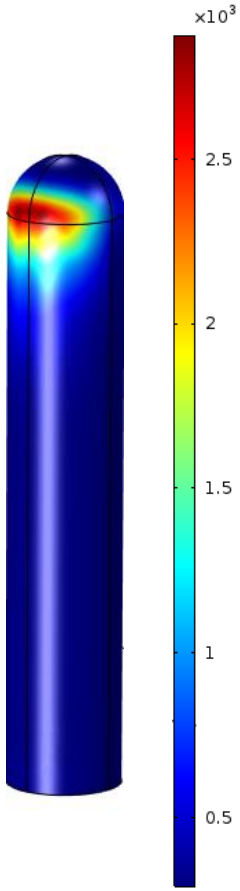
Activity at Tartu university focus mostly on analysis of stresses due to the laser pulse heating

Surface modifications appear on a tungsten tip in high electric fields in the area exposed to the femtosecond-laser impulse.

Laser impulse heats the electrons

Lattice heats via electron-phonon coupling

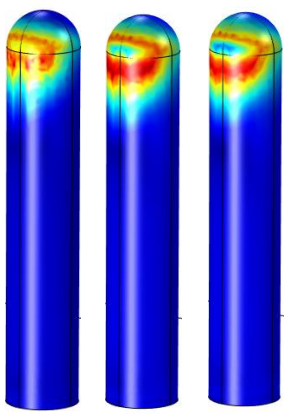
Laser heating creates massive thermal stresses



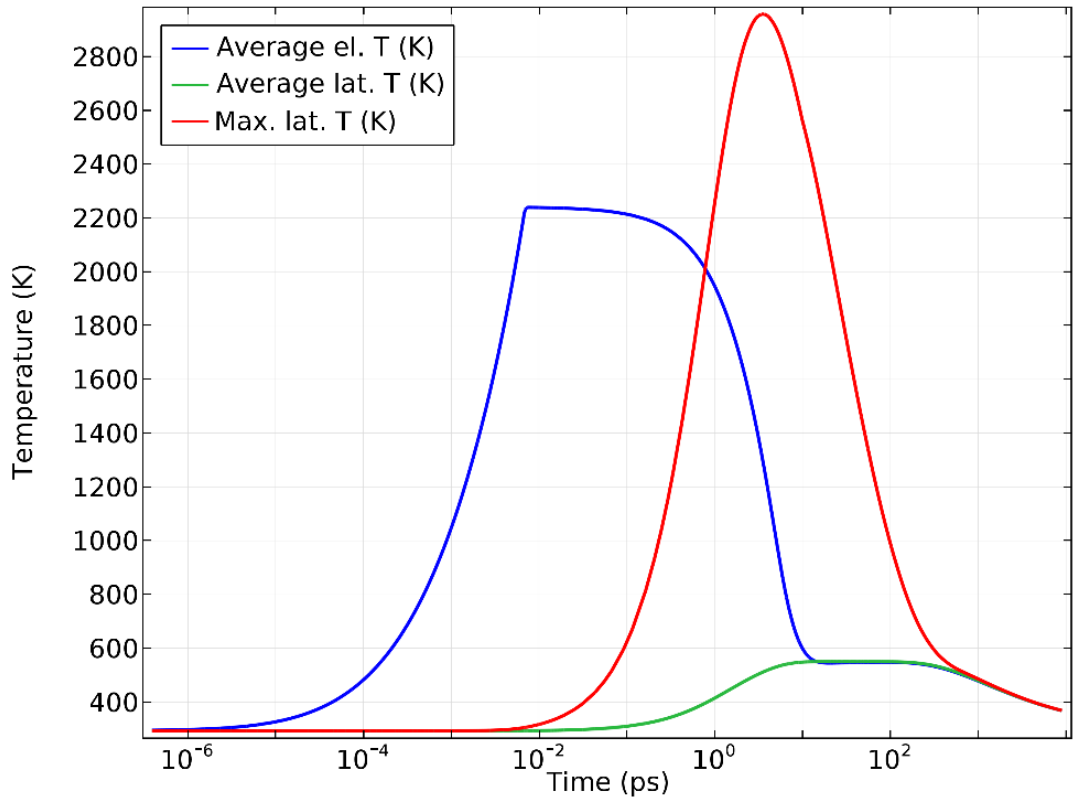
Asymmetric faceting effect on a laser-irradiated tungsten tip

Lattice temperature distribution at 5 ps, near lattice temperature peak

Von Mises stress due to lattice heating

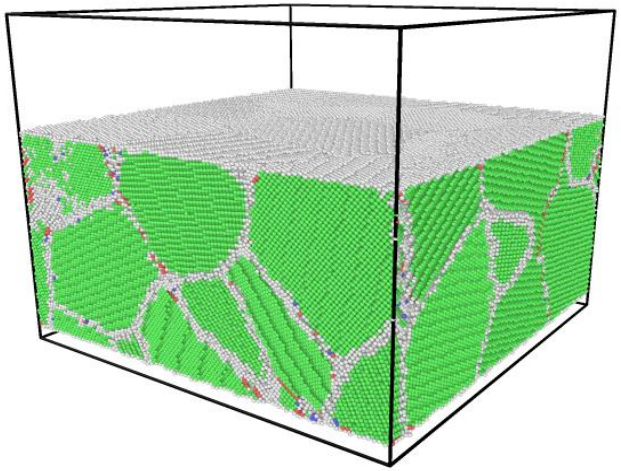


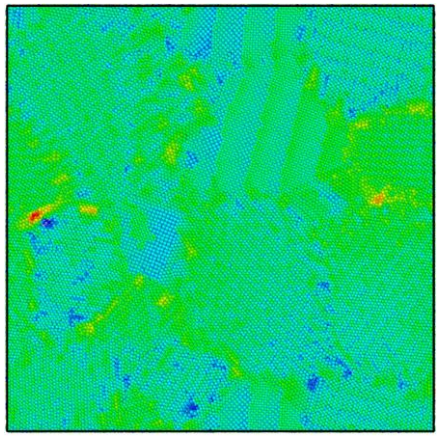
1 ps 2 ps 3 ps

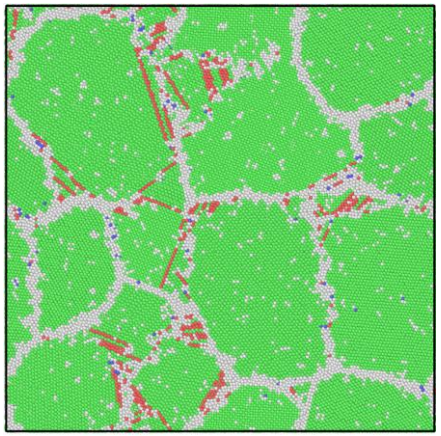


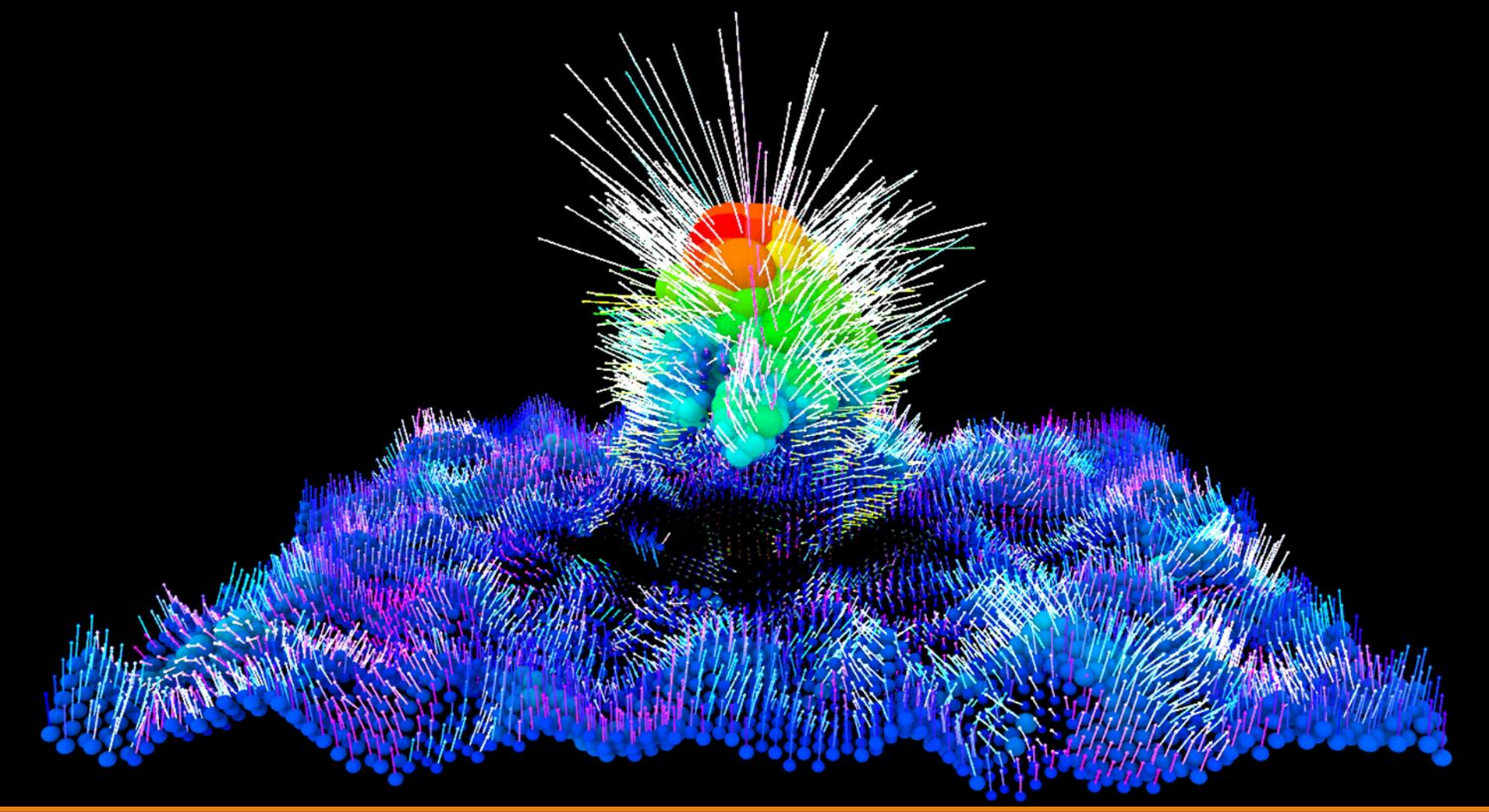
Polycrystalline copper surface deformations due to applied electric field

- Plastic response of polycrystalline surfaces
- Interaction of grain boundaries with a free surface in electric field
- Electric field is modelled as a force on the surface atoms perpendicular to the surface
- Preferential surface diffusion towards the intersections of grain boundaries with the surface









Thank you for your attention!