# Growth mechanism of a nano-protrusion on a tungsten tip under electric field

**by Ekaterina Baibuz***

Robert Aare**

Henrique Vázquez*, Hirofumi Yanagisawa***, Vahur Zadin*, Ville Jansson*, Flyura Djurabekova*

**** Department of Physics, Faculty of Science, University of Helsinki, Finland***

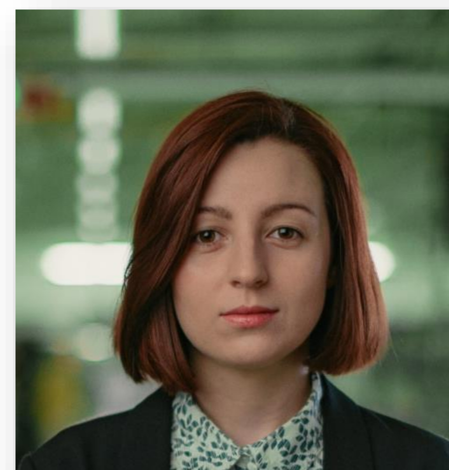
****** Intelligent Materials and Systems Lab

Institute of Technology

University of Tartu

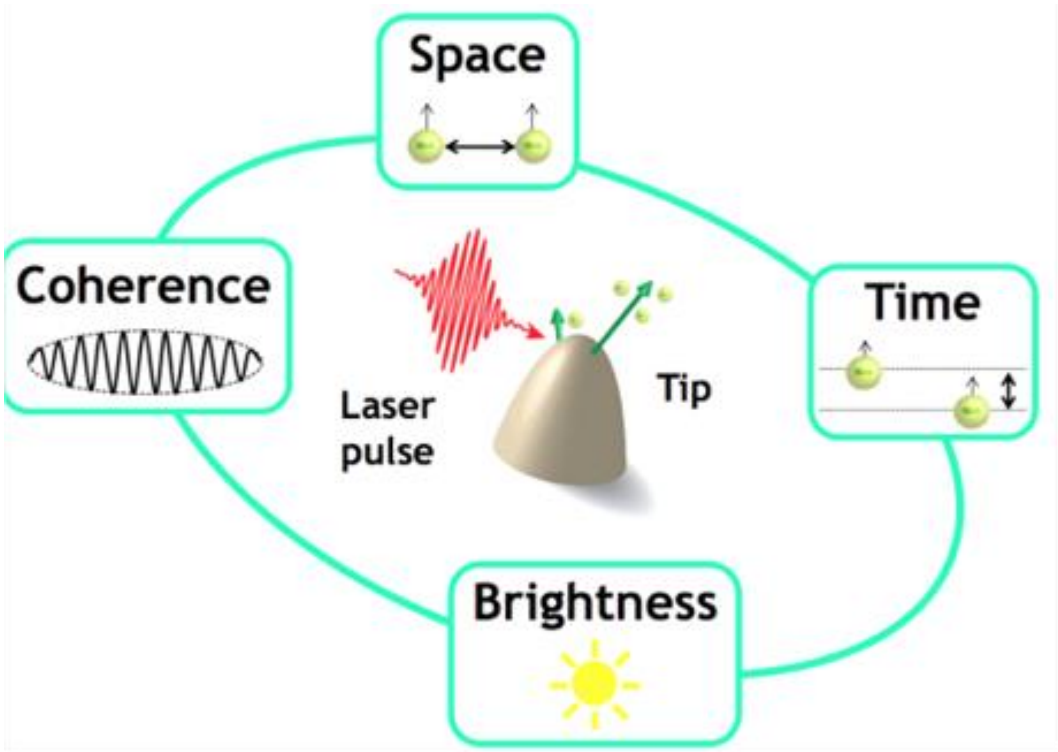
*** Ludwig-Maximilians-University of Munich

Munich, Bavaria, Germany

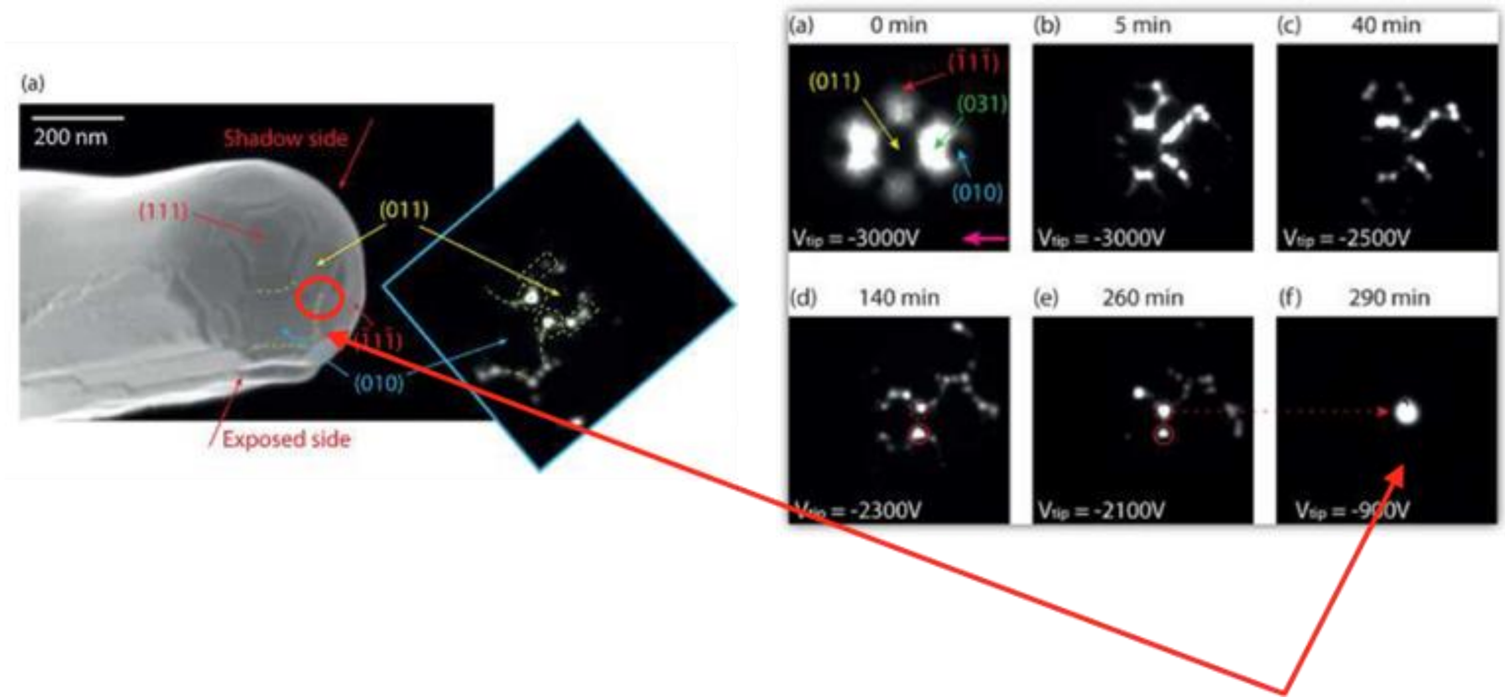


# W experiment overview

- 7 fs lase pulses
- field emission conditions



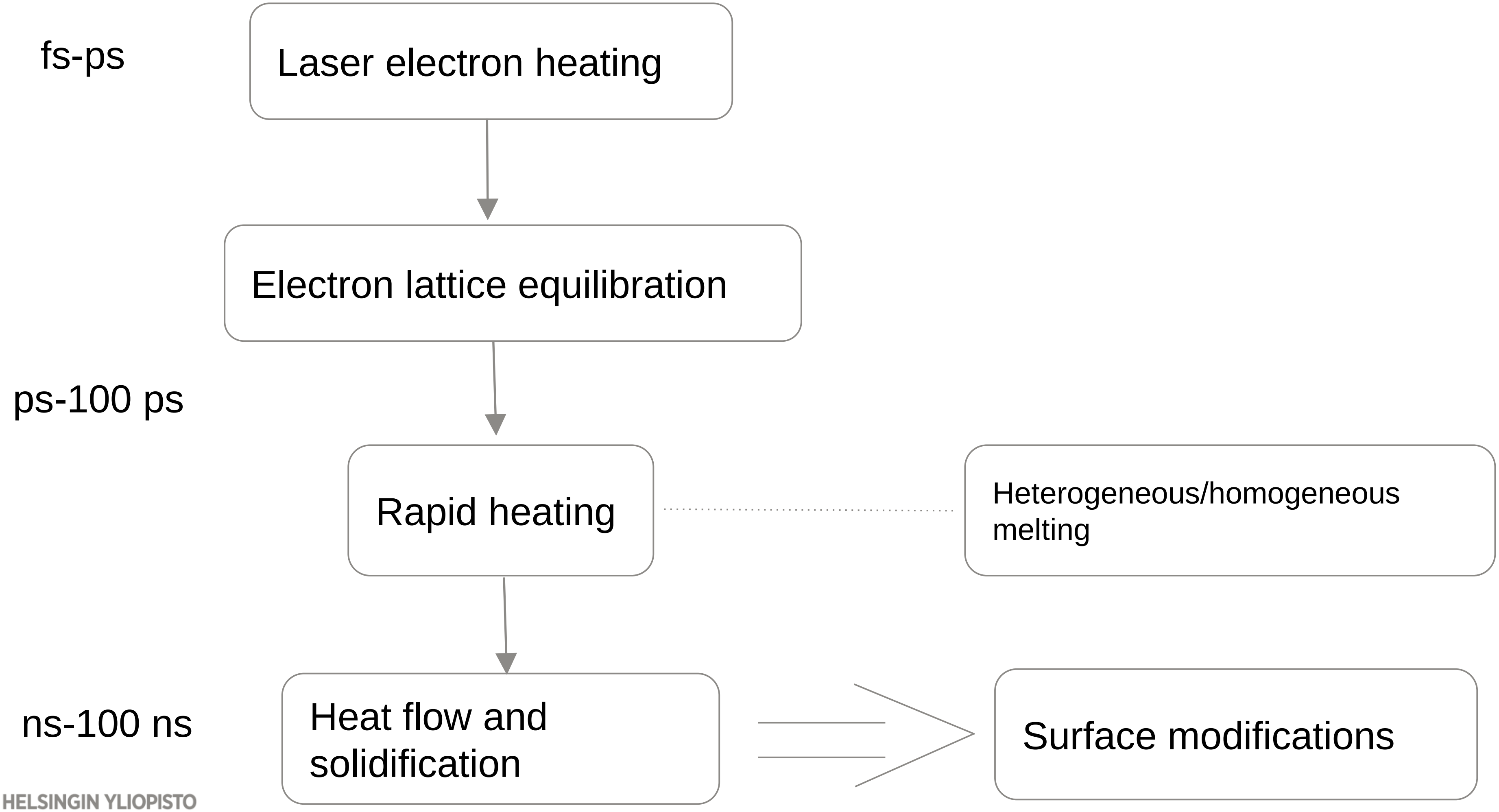
# W experiment overview




Laser heating + field emission conditions = growth of a nanotip after 5h of irradiation

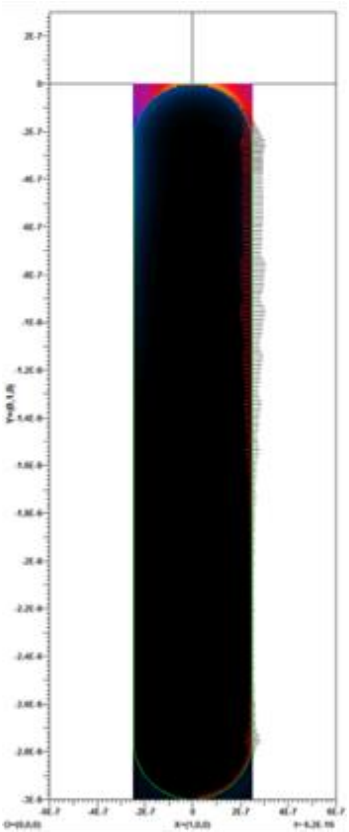
H. Yanagisawa, et al.APL Photonics(2016)

# Laser interaction with matter



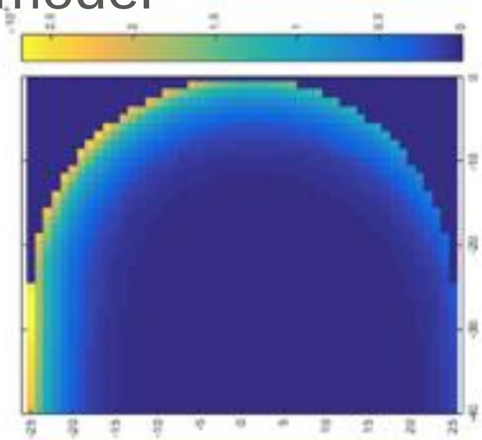
# Electromagnetic field propagation

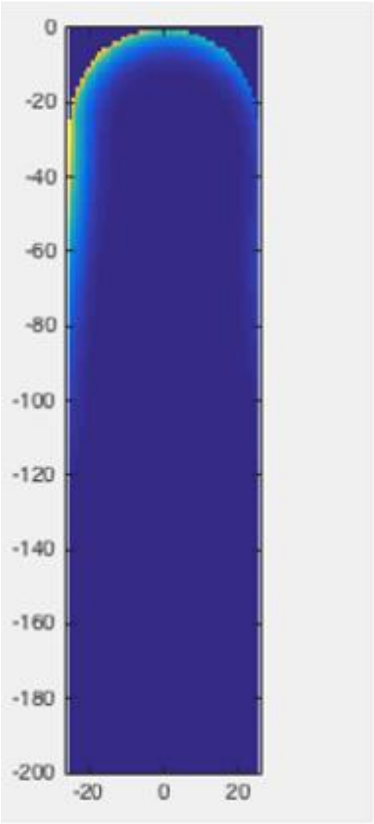
- OpenMaxWell software was used for solving Maxwell's equations
- Propagation of the electromagnetic field was obtained
- Laser was assumed as a planar wave



# Electromagnetic field propagation

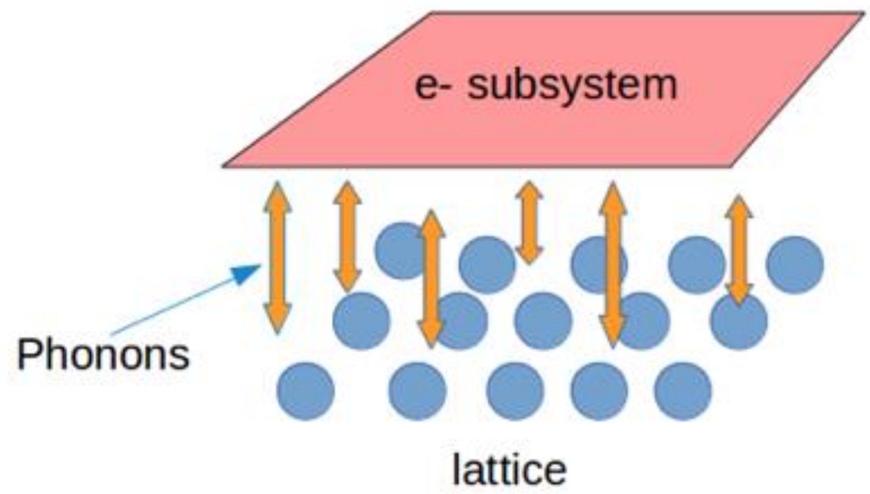
- Energy deposited on a tip by Joule heating
- Deposited energy was scaled to Gaussian laser pulse:
  - with peak of the pulse in the center of the tip
  - width of the Gaussian = half of the laser waist
- Deposited energy was used as an input for the Two Temperature model





# Two temperature model

- Two separate subsystems: electrons and lattice.
- Each subsystem is in thermal equilibrium.
- Subsystems exchange energy through electron–phonon interaction.

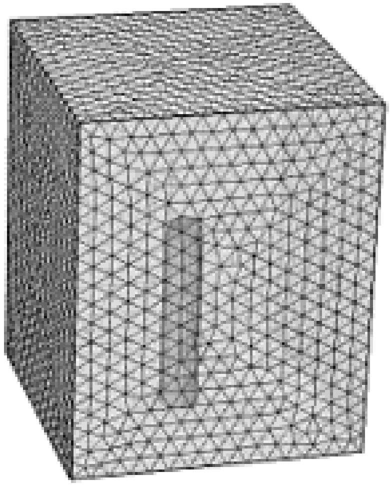


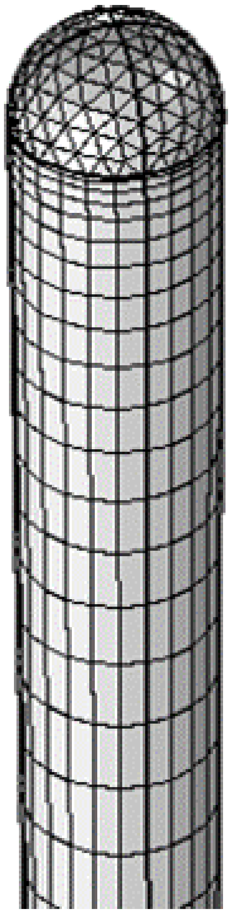

$$C_e \frac{\partial T_e}{\partial t} = \nabla \cdot (k_e \nabla T_e) - G(T_e - T_l) + A(\vec{r})$$

Te - electronic temperature, Tl - lattice temperature

# Finite Element Method(FEM)

- complex geometries simulated by subdividing into smaller, simpler parts=finite elements
- continuum method, i.e. no individual atoms
- fast and optimal
- TTM heat equations were solved with the FEM
- TTM was implemented in COMSOL Multiphysics FEM software

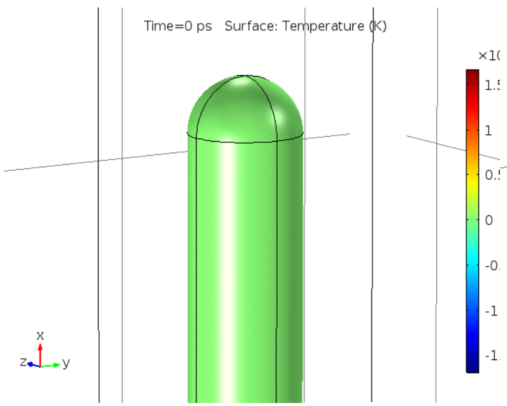




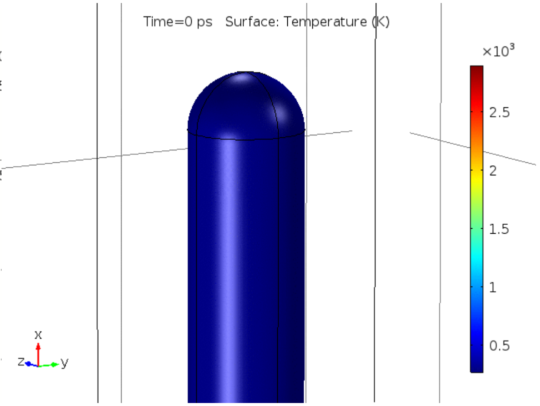
# Finite Element Method(FEM)

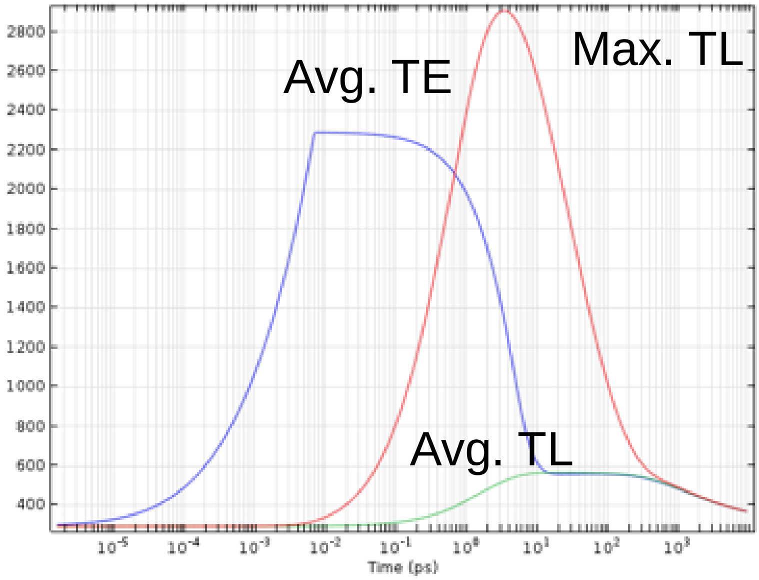
- Max temperature reached ~ 3000 K,
- Lattice temperature does not reach melting temperature without heat sources other than laser beam

Electronic temperature




Lattice temperature



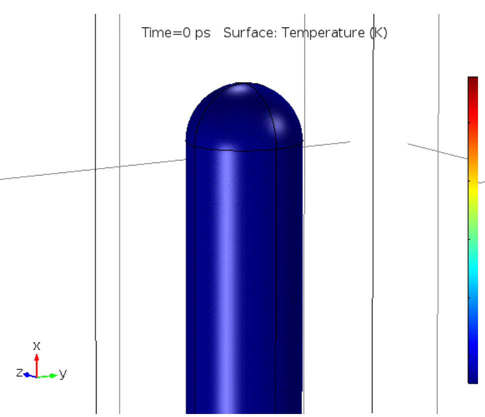




Temperature behaviour a fter the laser impulse; TL denoting lattice temperature, Te electroni c temperature.

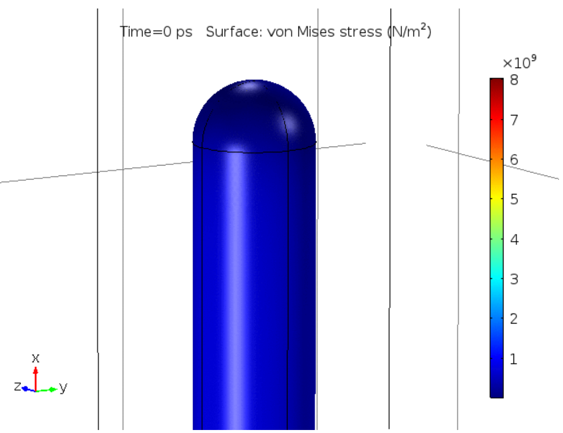
# FEM results. Stresses

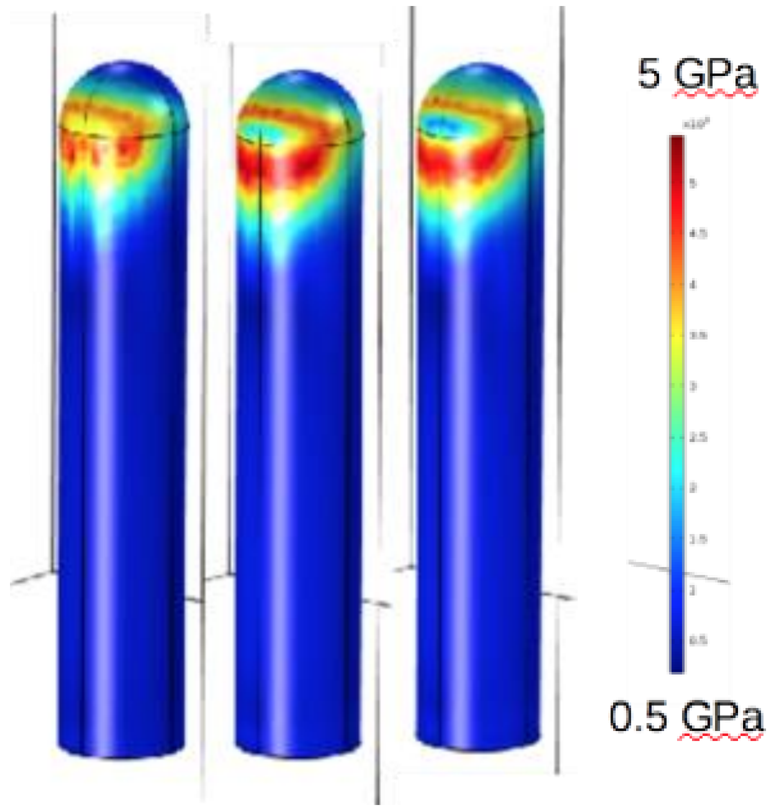
- Von Mises stress wave can be observed as energy is transferred from electrons to the lattice
- laser heating creates massive thermal stresses

Lattice temperature



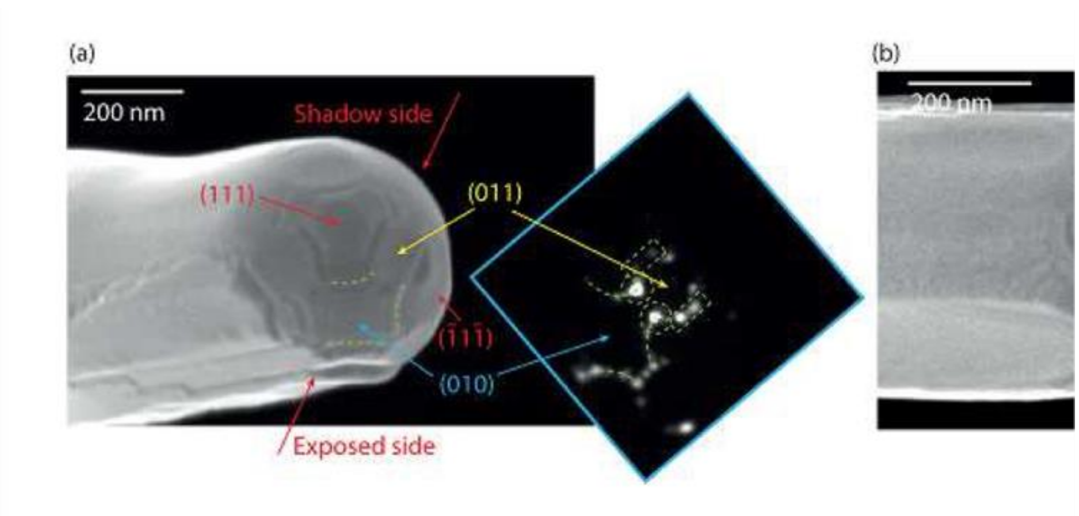

Stress



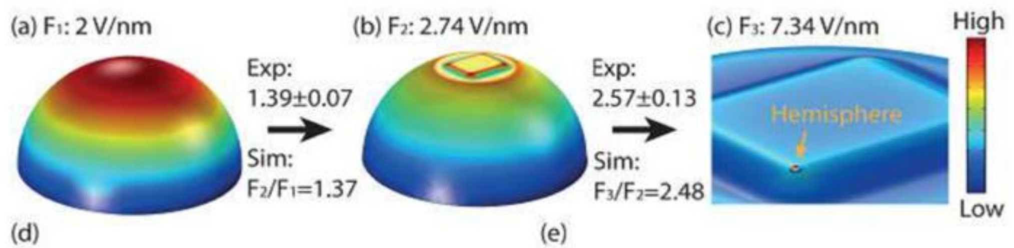




1 ps 2 ps 3 ps

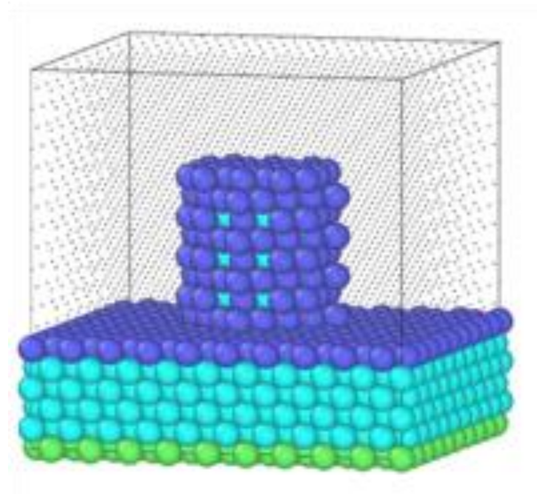
# Nano-protrusion on a plateau




- Nanotip growth happens via surface diffusion
- To see a diffusion on a plateau, Kinetic Monte Carlo model is needed



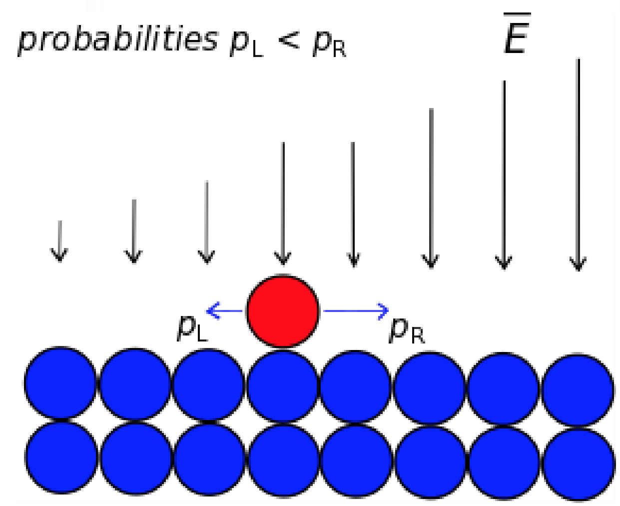
# Kinetic Monte Carlo model under electric field



- Rigid lattice is assumed E
- Thermally activated jumps to vacant 1nn sites:

$$\Gamma = \nu e^{\left(\frac{-E_m}{k_b T}\right)},$$

where $\nu$ is the attempt frequency, $k_b$ - Boltzmann's constant, $T$ - the temperature, and $E_m$ - the migration barrier that an atom needs to overcome in order to make a jump.

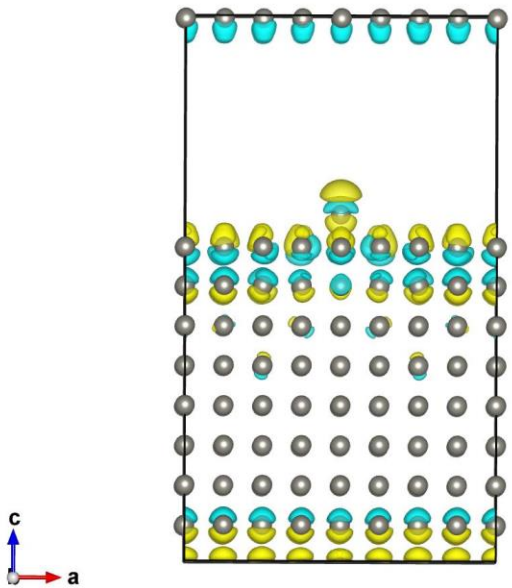



- Adatoms on a surface become dipoles under electric field
- Migration barriers are affected by electric field
- Diffusion will be biased towards higher fields
- Bias is defined by the adatom's polarisability

More details in V. Jansson's talk

# DFT calculations of W adatom on W

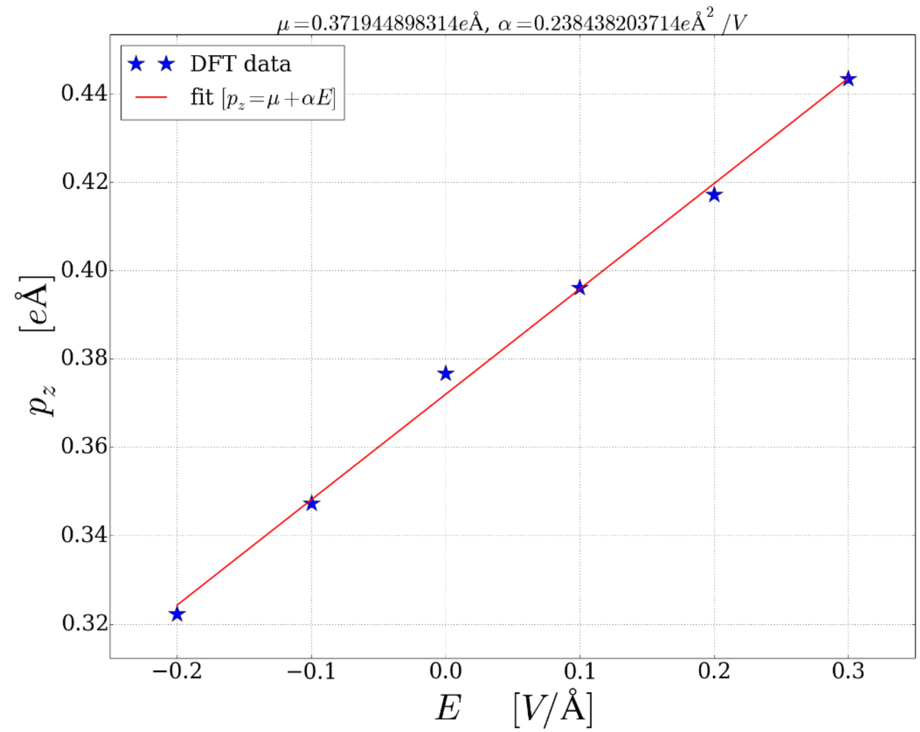
Charge induced by electric field:




Accumulation of electrons by electric field

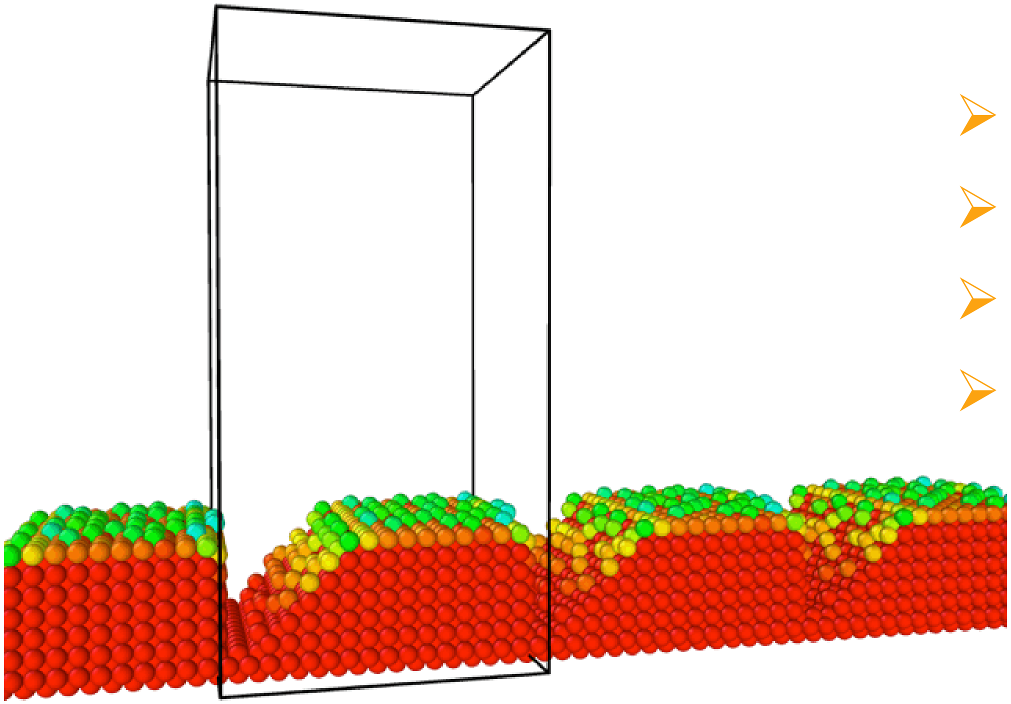
Depletion

Dipole moment vs. applied electric field:




VASP software was used

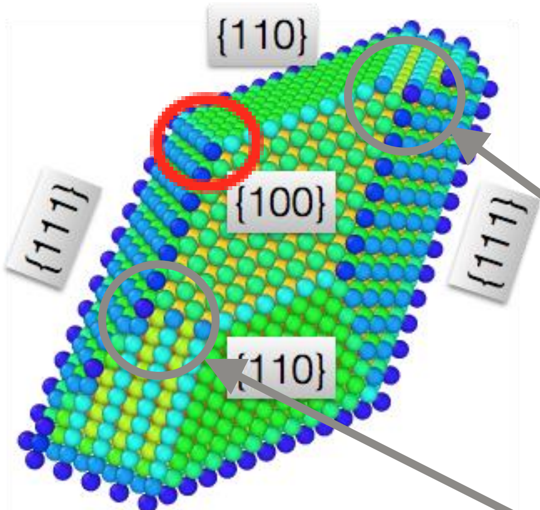
# KMC results

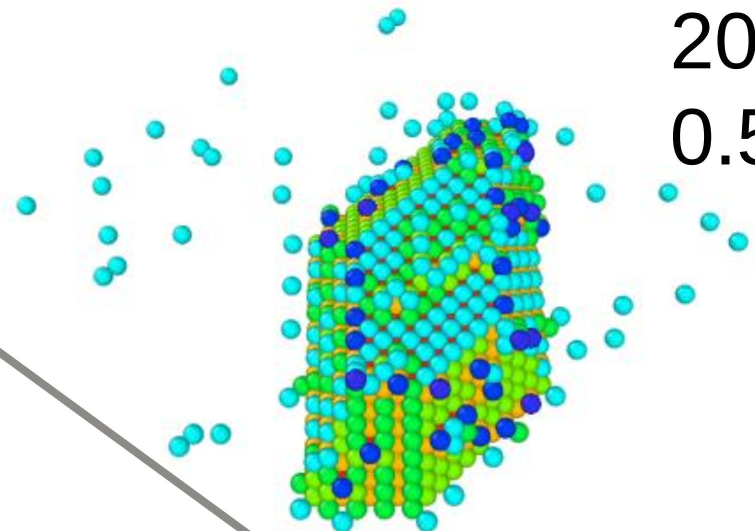


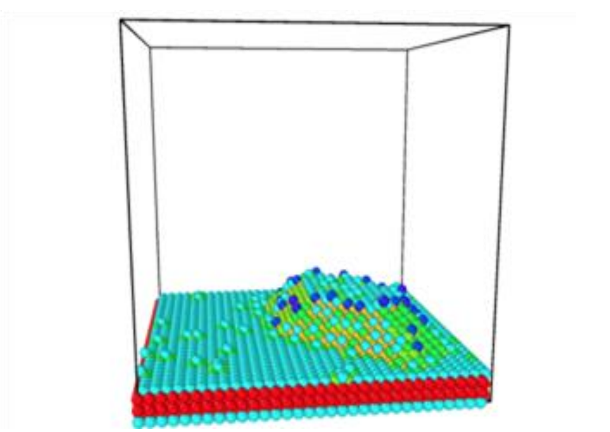
- Electric field solver HELMOD
- KMC code Kimocs
- 2500 K
- 1.0 GV/m
- Time scale ~ 0.1 μs

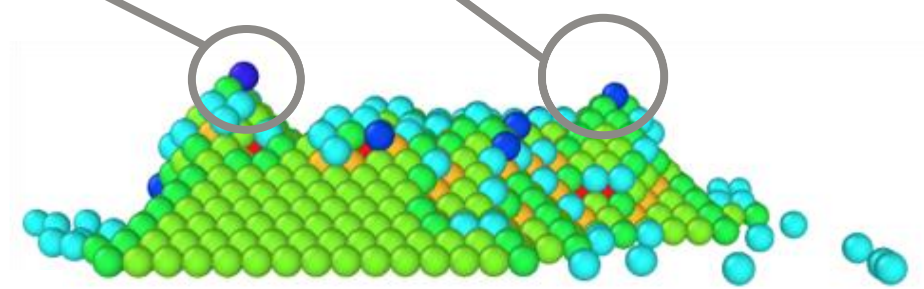
# Nano-protrusion growth on a plateau KMC results

2000 K
0.5 GV/m



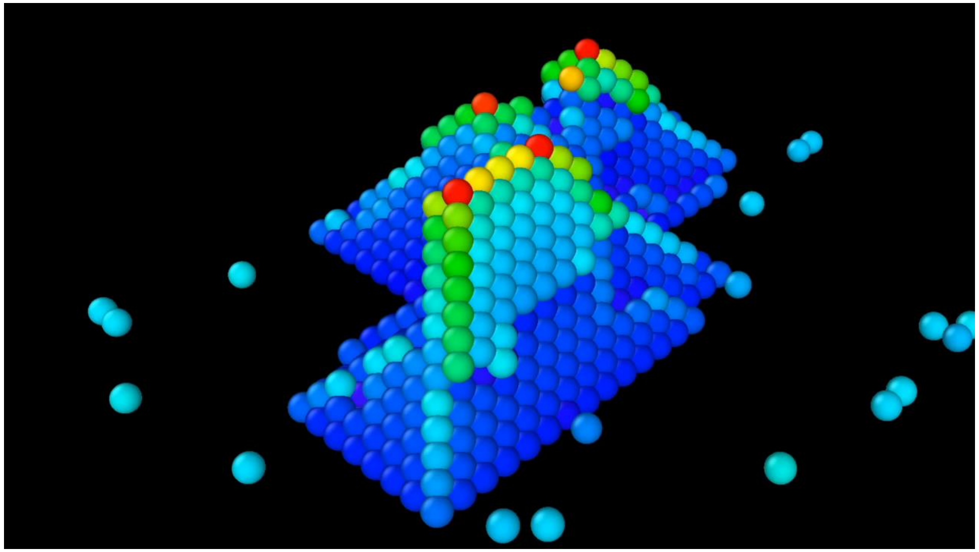




# Plateau. KMC results

- Plateau reorganises in ~ 1μs
- Atoms form closed-packed {111} facets
- Nano-protrusions grow between {111} facets
- Large system should be studied
- The system size was limited by HELMOD code

2500 K 0.5 GV/m Charge distribution:



Next Step: study large plateau with recently developed code FEMOCS.
More details in M. Veske's talk

# Summary

- FEM simulations coupled with TTM showed
  - Lattice temperature does not reach melting temperature without heat sources other than laser beam
  - Laser heating creates massive thermal stresses
  - Next step: include emission currents and Nottingham effect
- KMC simulations show growth if nano-protrusions on the edges between facets
  - Next step: study large plateau in KMC+FEMOCS