Tungsten under femtosecond laser irradiation Emission currents, thermal and mechanical behaviour

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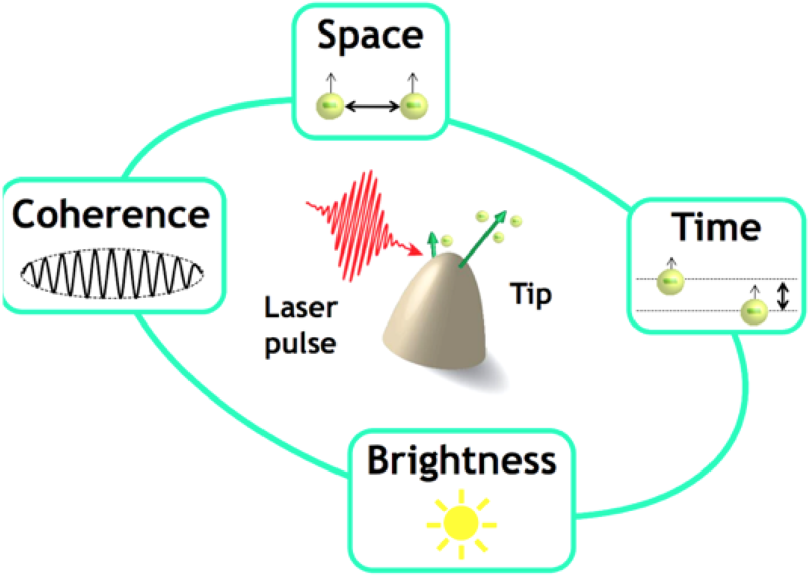
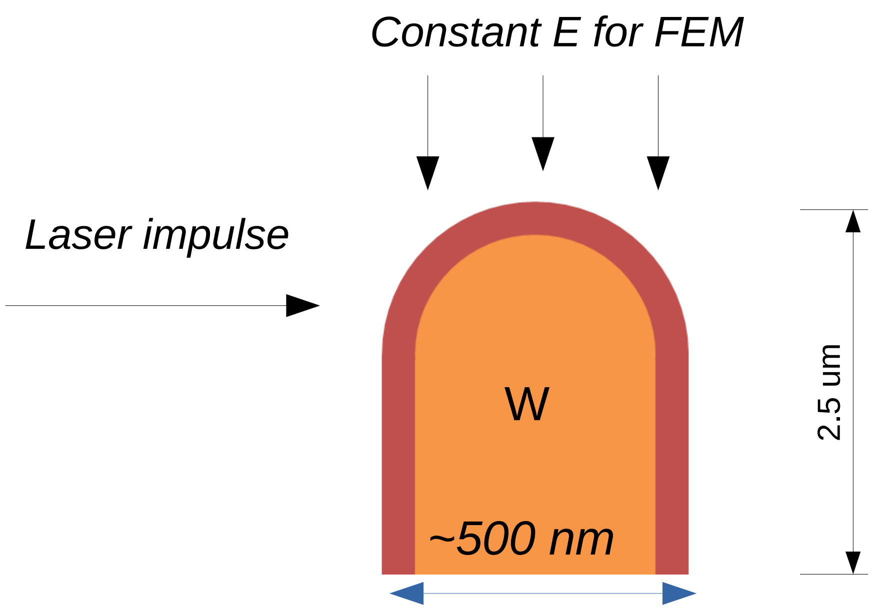
The experimental setup

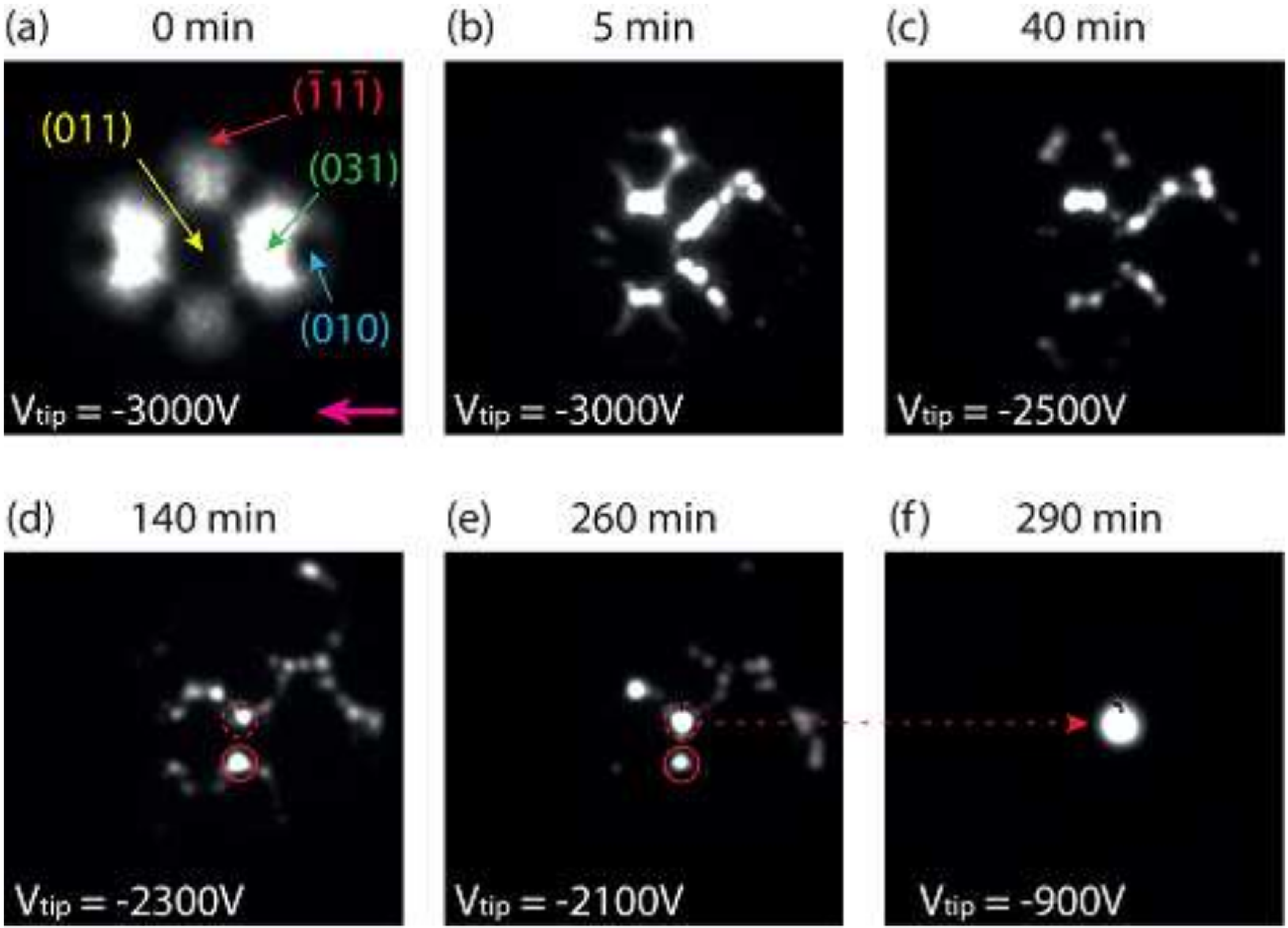
- Femtosecond-scale pulses with nominal beam power 180 mW
- Pulse interval 10 ns
- Constant monitoring of FEM picture, occasional SEM imaging





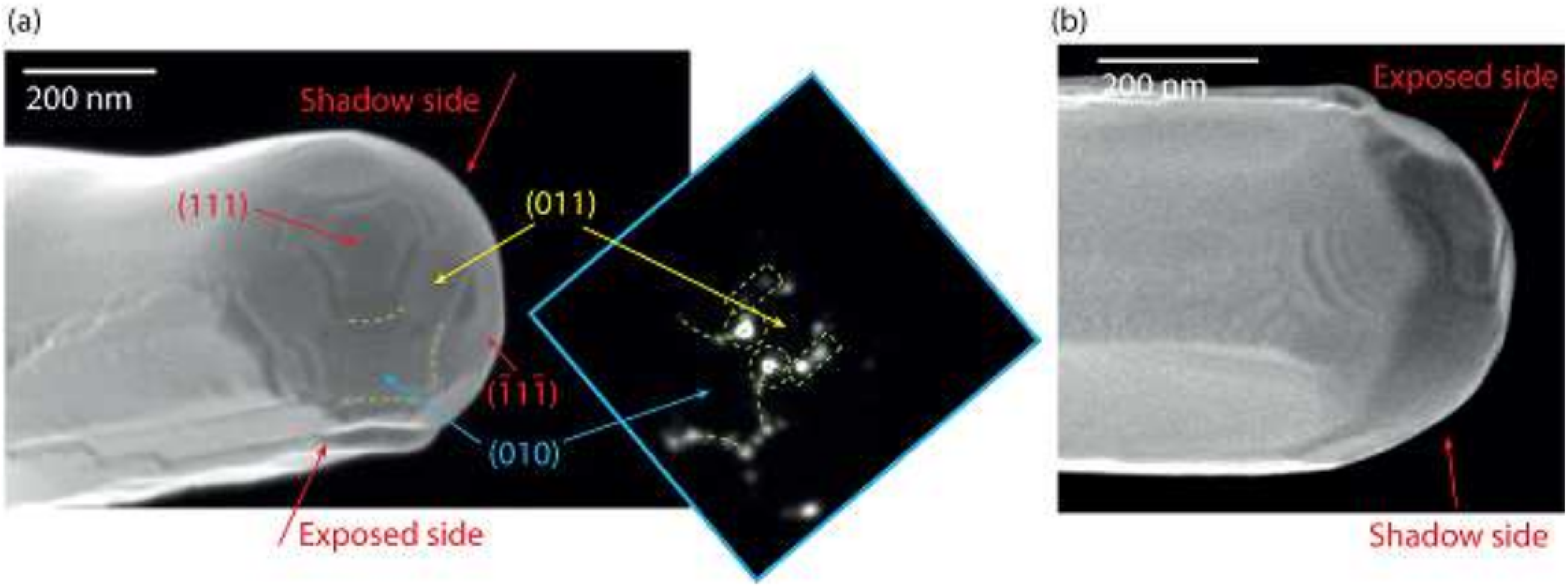
H. Yanagisawa et al., APL Photonics (2016)

The field emission transformation



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

The faceting as seen on SEM images



The faceting may create nanotips along the ridges formed between separate facets. After ***heating*** *up to 80% of the melting temperature,* ***facets disappear****, making the experiment* ***repeatable.***

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

Modeling the experiment

- Different phenomena to consider:
  - Electric field (for FEM and from laser impulse)
  - Emission currents
  - Laser-tungsten interaction
  - Heat deposition and propagation
  - Thermal stresses
  - Quantum effects on surface
  - Surface diffusion*

Mathematical formulation

Heat equations:

$$\rho C_L \frac{\partial T_L}{\partial t} + \rho C_L \boldsymbol{u} \cdot \nabla T_L + \nabla \cdot (-k_L \nabla T_L) = Q_L$$

$$C_e \frac{\partial T_e}{\partial t} + C_e \boldsymbol{u} \cdot \nabla T_e + \nabla \cdot (-k_e \nabla T_e) = Q_e$$

Heat sources:

$$Q_1 = g(T_e) \cdot (T_L - T_e)$$

$$Q_2 = -\sigma T^4$$

$$Q_3 = \mathbf{J} \cdot \mathbf{E}$$

$$Q_4 = \Delta E_e J$$

Laser EM-field:

$$\nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t}$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

$$\nabla \cdot \mathbf{D} = \rho$$

$$\nabla \cdot \mathbf{B} = 0$$

Emission current density:

$$J_{GTF}(F, T) = A_{RLD} T^2 N\left(\frac{\beta_T}{\beta_F}, \beta_F (E_0 - \mu)\right)$$

Thermal and electrostatic stress:

$$T_{ij} = \epsilon_0 \left(E_i E_j - \frac{1}{2} \delta_{ij} E^2\right) + \frac{1}{\mu_0} \left(B_i B_j - \frac{1}{2} \delta_{ij} B^2\right)$$

$$S = s_0 + C : (\epsilon - \epsilon_0 - \epsilon_{th})$$

$$\epsilon_{th} = \alpha (T - T_{ref})$$

$$S = F^{-1} P \qquad s = J^{-1} P F^T \quad J = det(F)$$

$$p = -\frac{1}{3} trace(s) = \frac{-s_{kk}}{3}$$

$$s_d = s + pI$$

$$J_2(s) = \frac{1}{2} s_d : s_d$$

$$s_{Mises} = \sqrt{3 J_2(s)}$$

Static EM-field:

$$\nabla^2 V = 0$$

$$\mathbf{E} = -\nabla V$$

Modeling the experiment

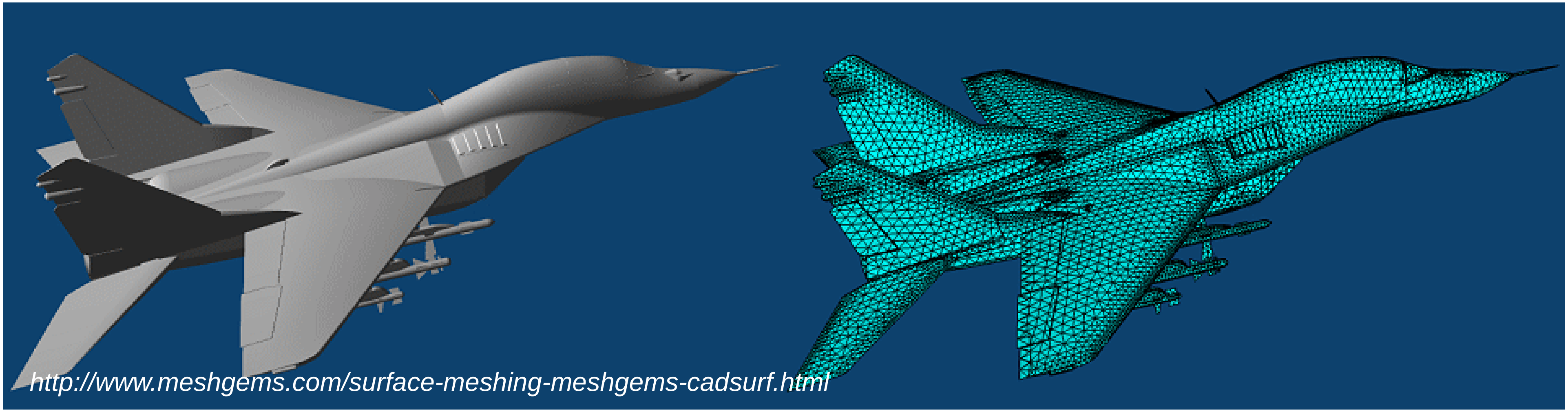
Different methods are needed to describe the many underlying phenomena properly:

- FEM+MD for evaluation of the emission currents, thermal and mechanical behaviour
- KMC with E-field and MD for surface diffusion and tip growth
- DFT for calculation of E field induced charges
- ...others added, as needed

There is no way around multiscale modeling

The finite element method

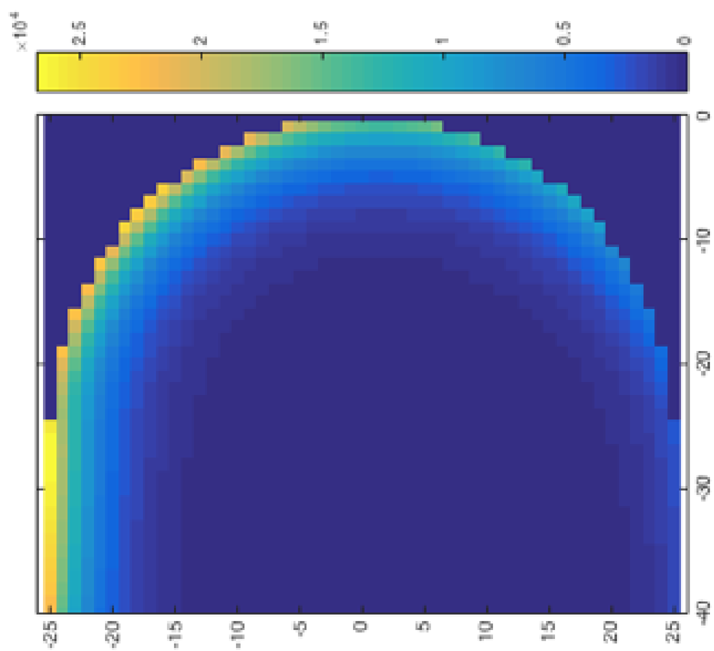
- Allows simulating complex continuum geometries by subdividing geometry into small easily described parts (finite elements)
- Computationally very efficient
- The models described hereafter are created with COMSOL MultiPhysics
- **We do not see atoms!**

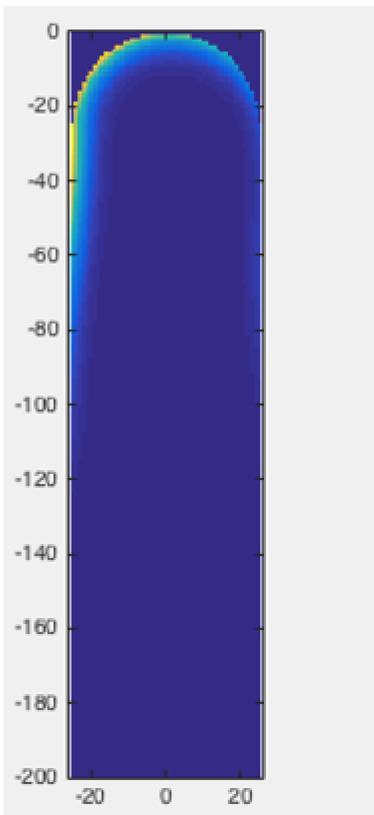


Laser energy deposition

- Laser modelled as energy deposition rate
- Calculated using OpenMaxwell
- Energy scaled to fit a Gaussian pulse, peak of the pulse set to hit the center of the tip

Deposited beam energy is used as direct input for the heat equation.





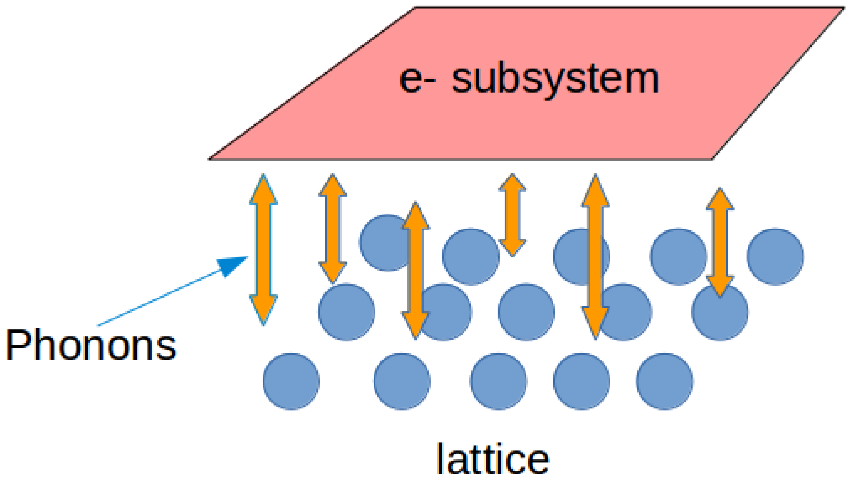
OpenMaxwell calculations by Henrique Vázquez, Helsinki

The two-temperature model

The fs-timescale induces a thermal inbalance between electrons and atoms

Both subsystems are otherwise in thermal equilibrium

Energy exchange between atoms and electrons takes place via **electron-phonon coupling**

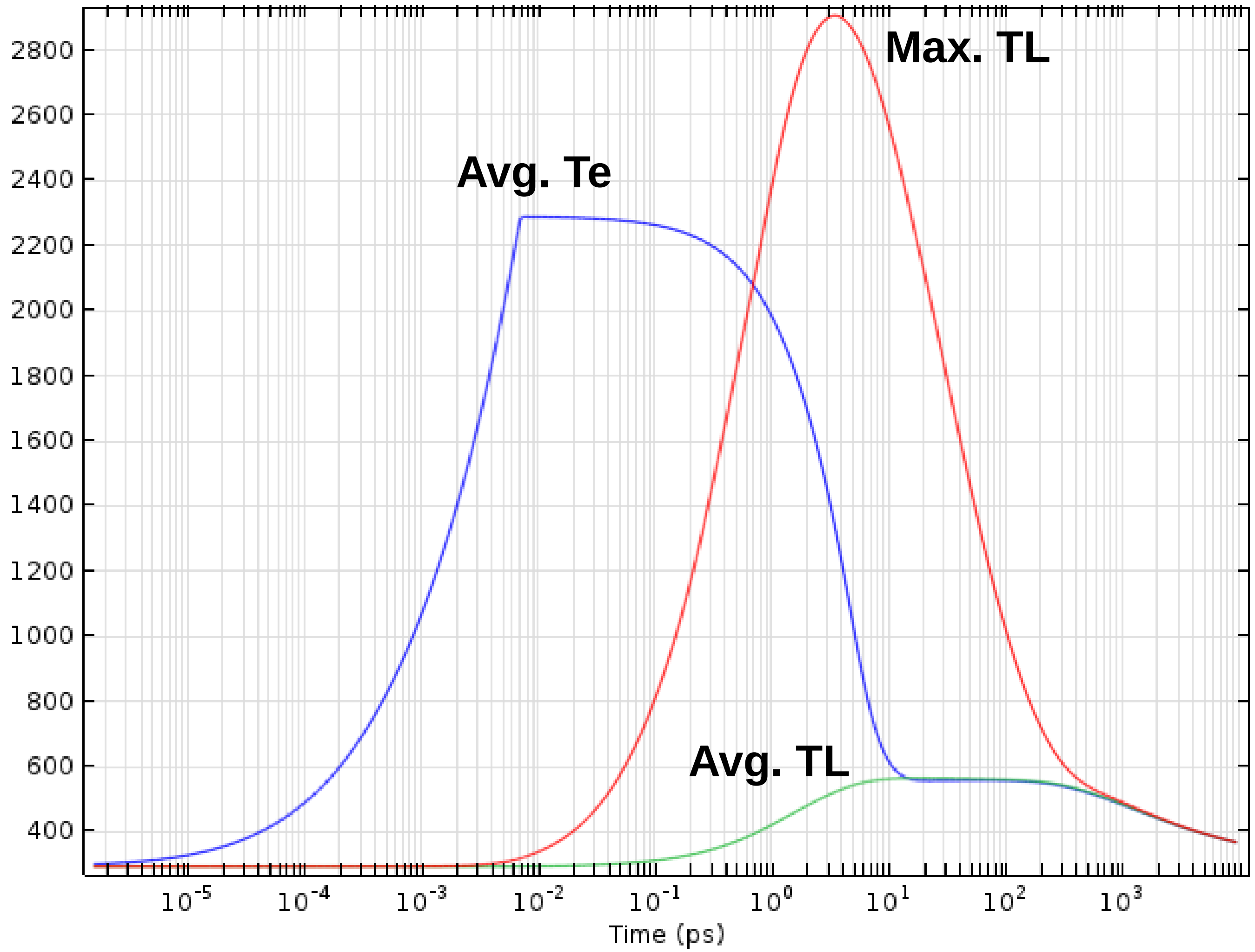


http://dx.doi.org/10.1103/PhysRevB.80.035415

Normal TTM temperature behaviour

Maximum lattice temperature reaches **3050 K**

Melting point for W is **3695 K**



Time in log scale!

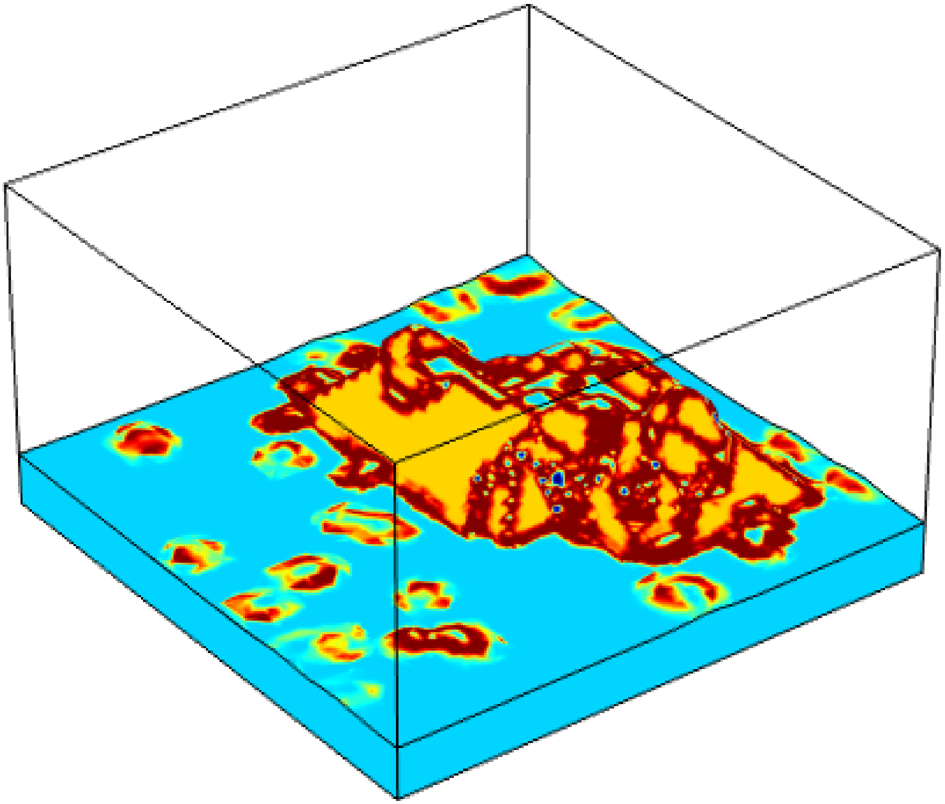
Doubling the laser energy deposition takes the maximum lattice temperature to ~5100 K. **1.25** times greater energy deposition results in reaching melting temperature.

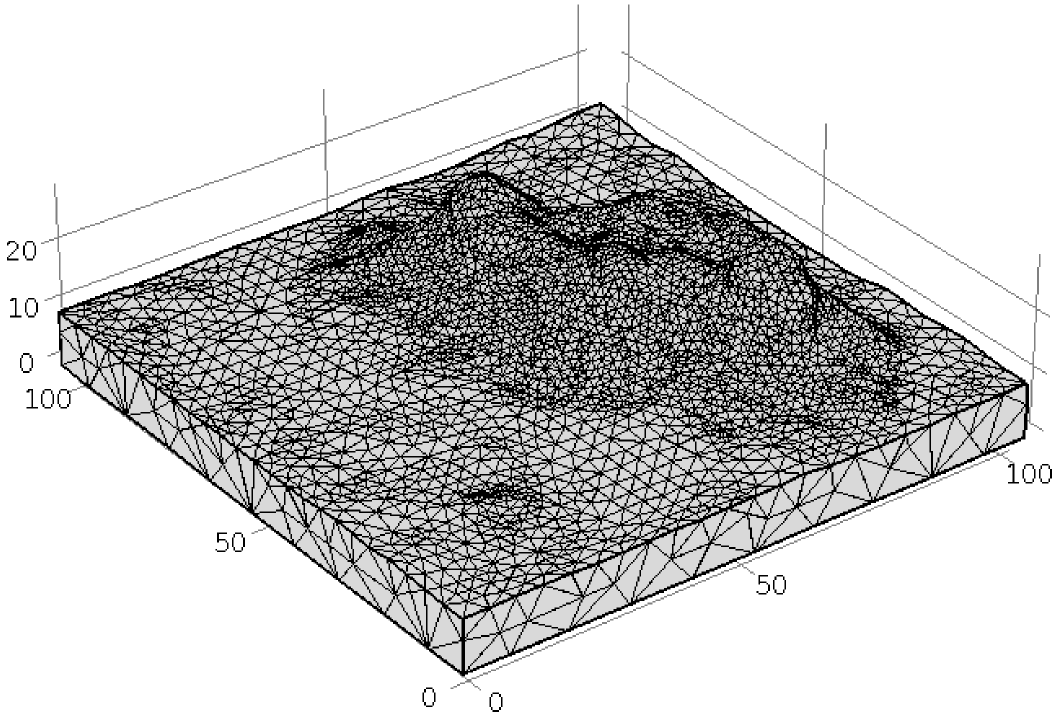
Emission currents

- The electric field at the apex of the tip is estimated to be a few GV/m – electrons can easily tunnel out of the surface
- Emission currents modelled using the **General Thermal Field equation**
- **Nottingham effect** and **Joule heating** give additional heat effects
- Emission currents have a dependence on **crystal surface orientation** (work function)

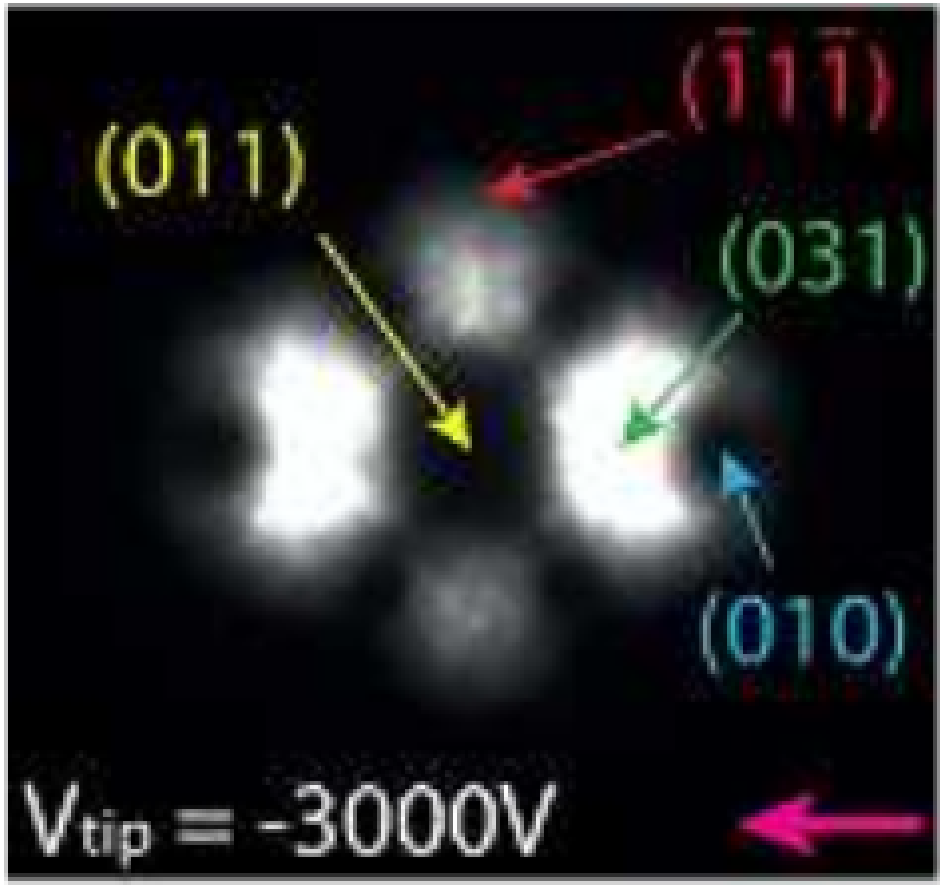
Crystal surface orientations

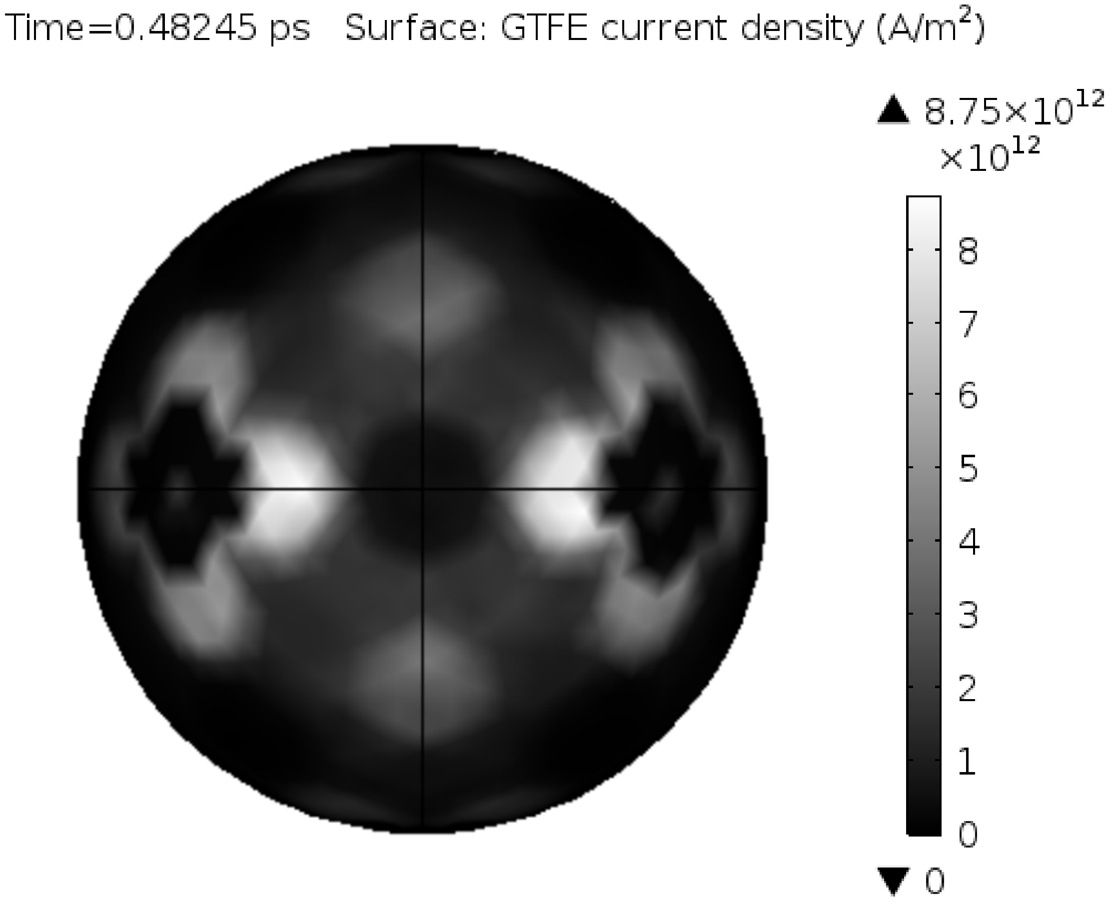
If we choose the correct coordinate base in FEM, we can calculate the crystal surfaces from surface normals – Miller indices





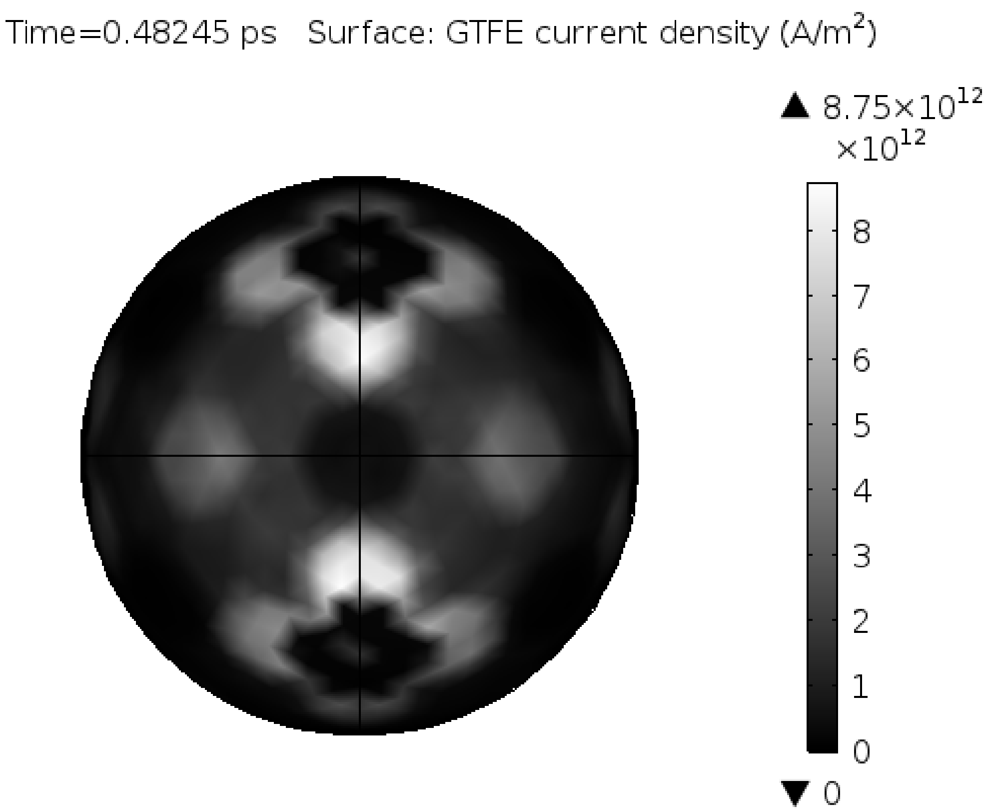
Crystal surface orientations for EC

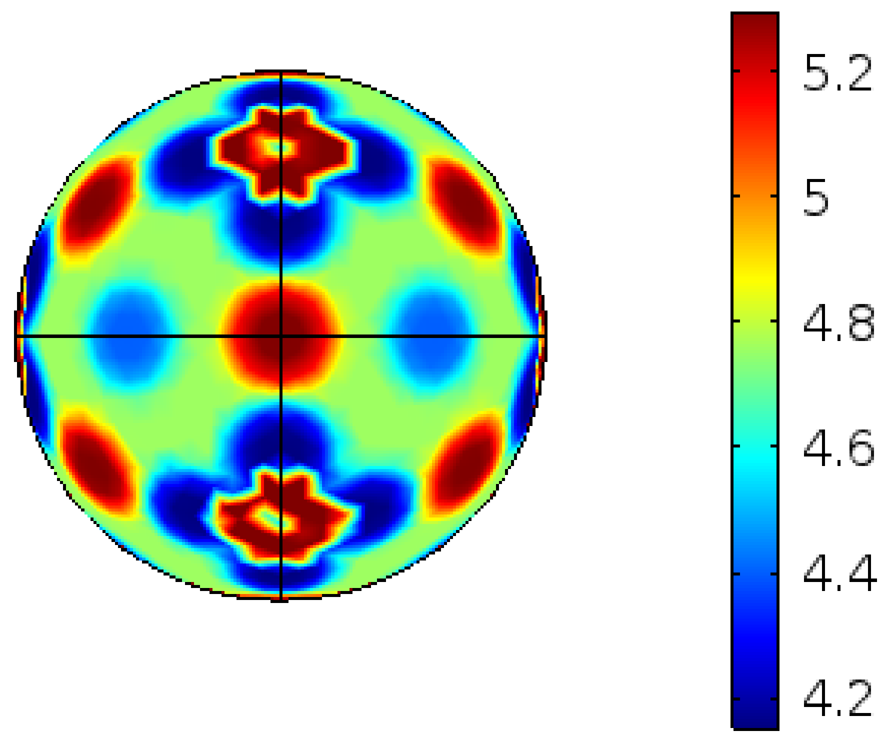




For a smooth hemispherical tip, with the crystal surface dependent emission currents, we have excellent agreement with the experimental measurement.

Work function and emission currents





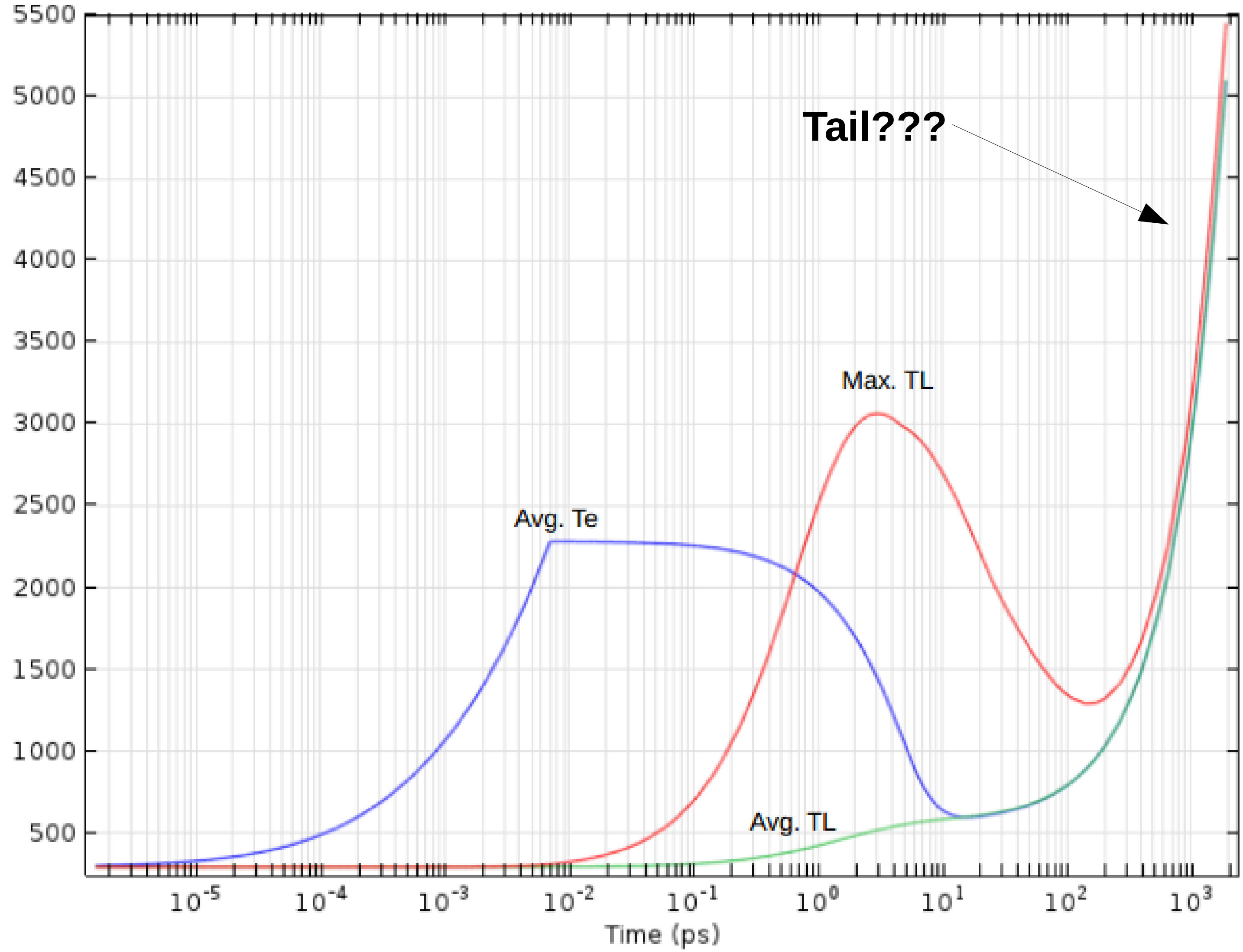
It’s easier for the electrons to tunnel out of the areas, where the surface work function is lower.

Temperature behaviour with EC

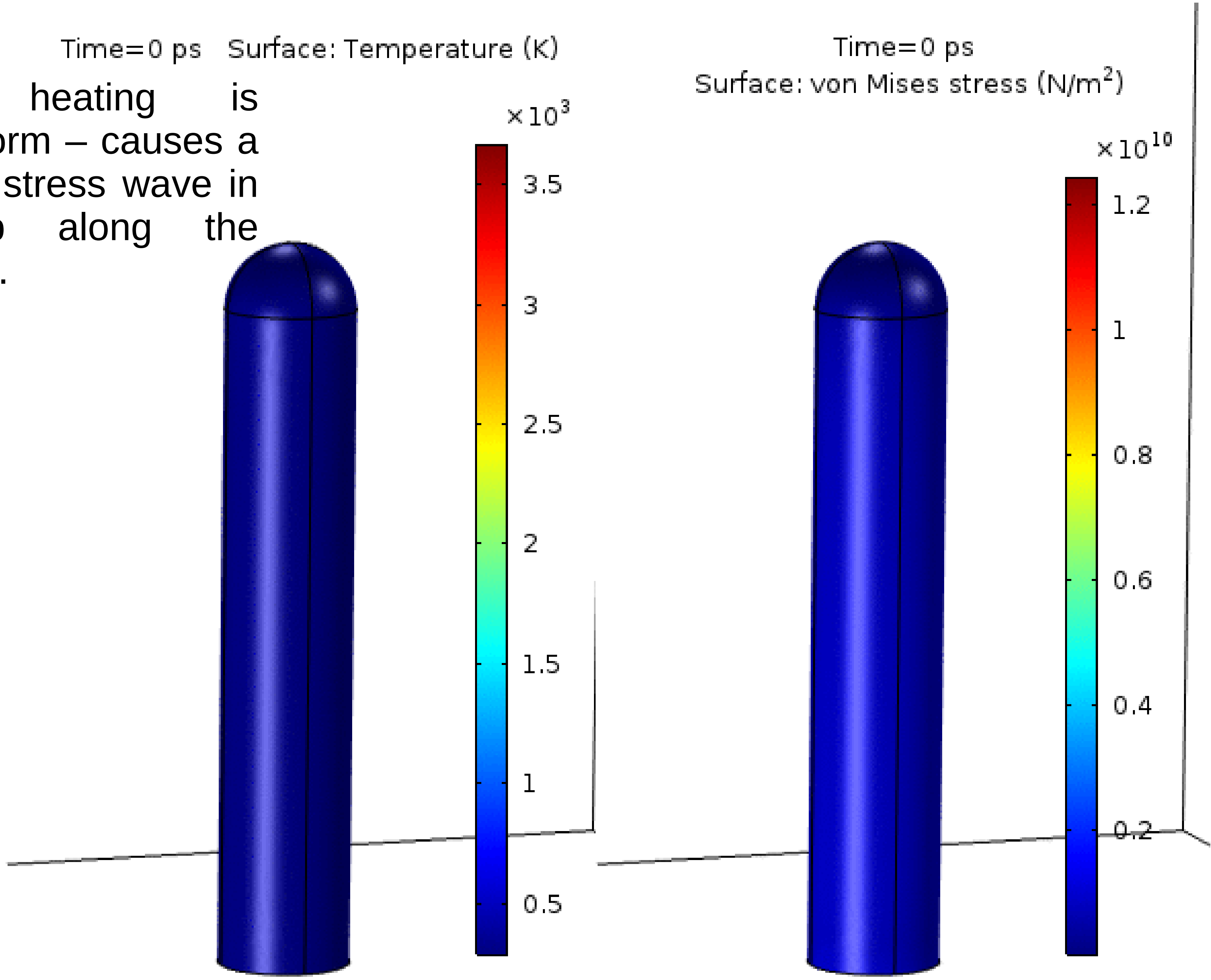
Additional thermal effects go into a feedback loop, the tip vapourizes.

This is because **space charge screening** is not taken into account.

Given the upper limit of the EF set by the SCS from GETELEC, we have shown that the heat overflow is avoided.



Laser heating is nonuniform – causes a thermal stress wave in the tip along the gradient.

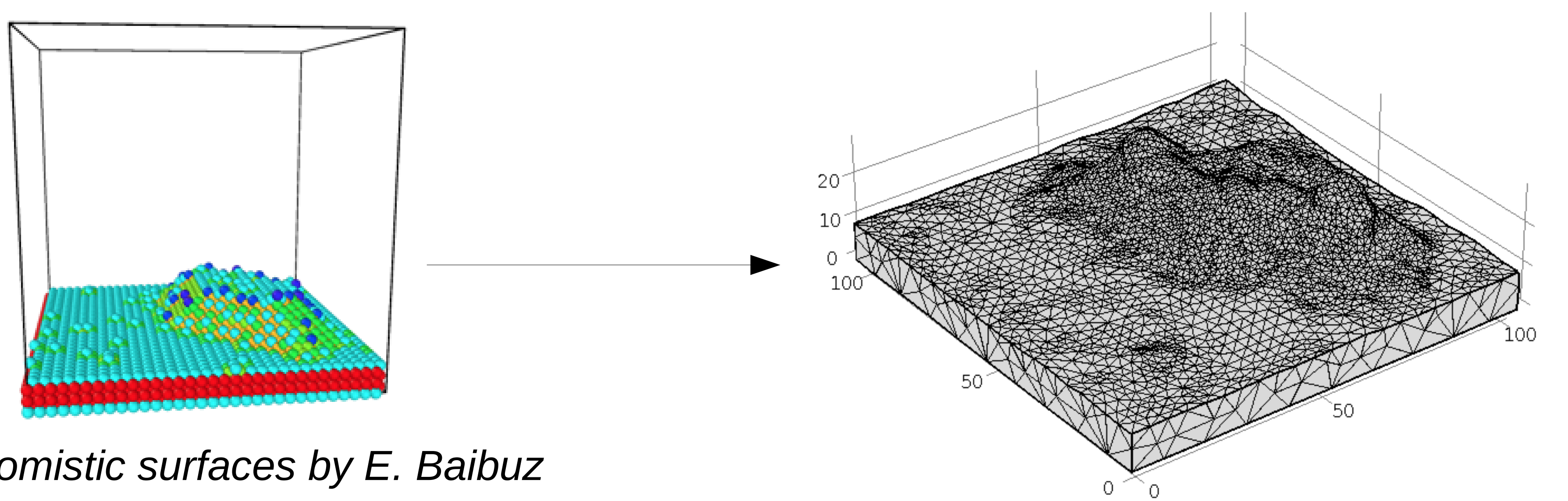


Stressful stress

- We see stresses, that should give plastic deformations (Gpa scale)
- MD simulation using the temperatures reached show nothing interesting – no notable dislocations nor tip growth
- Stress analysis becomes significantly more complex with partially melted tip

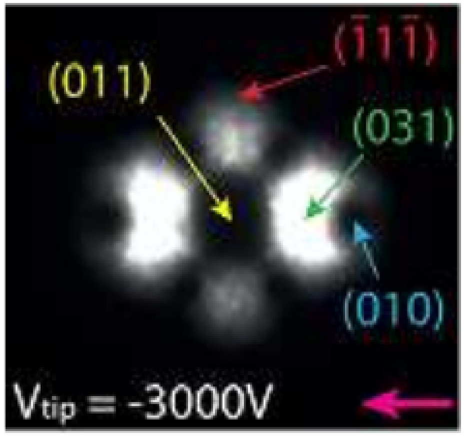
MD-FEM-KMC hybrid analysis

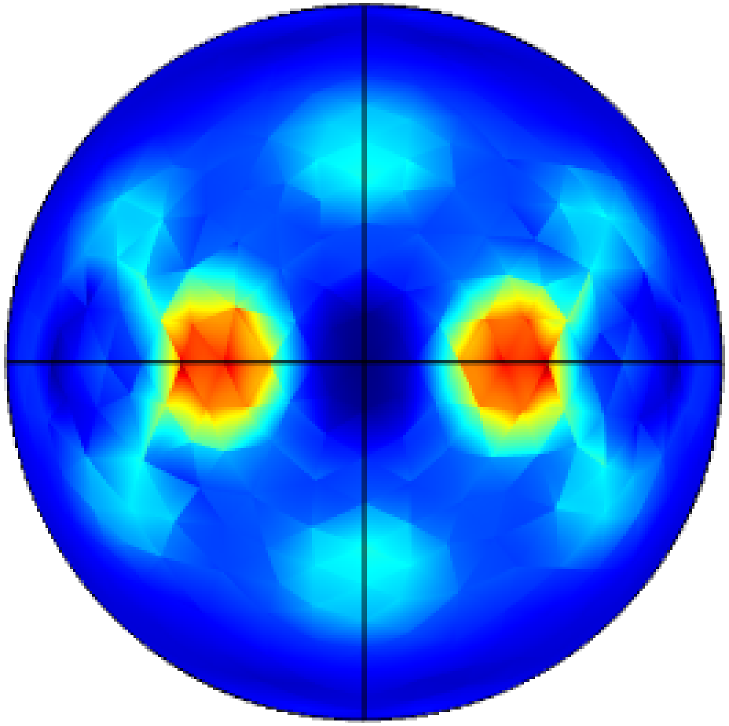
- Continuum models cannot show surface faceting and tip growth directly
- Molecular dynamics and Kinetic Monte Carlo simulations are used for atomistic simulations
- Atomistic surface is converted into a continuum surface using **screened Poisson surface reconstruction**



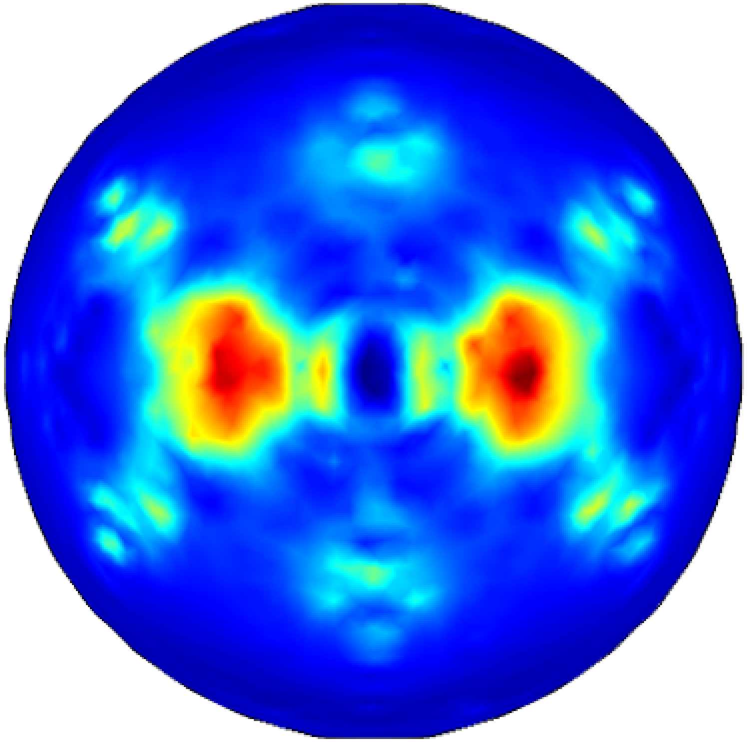
Atomistic surfaces by E. Baibuz

Emission patterns for MD surfaces



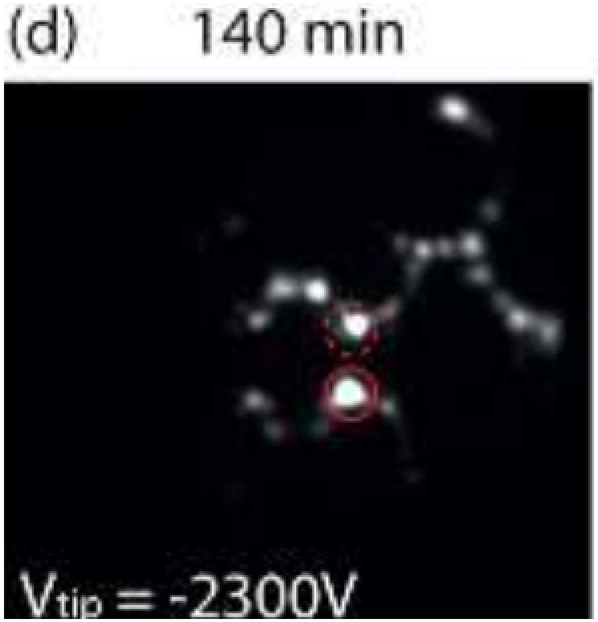


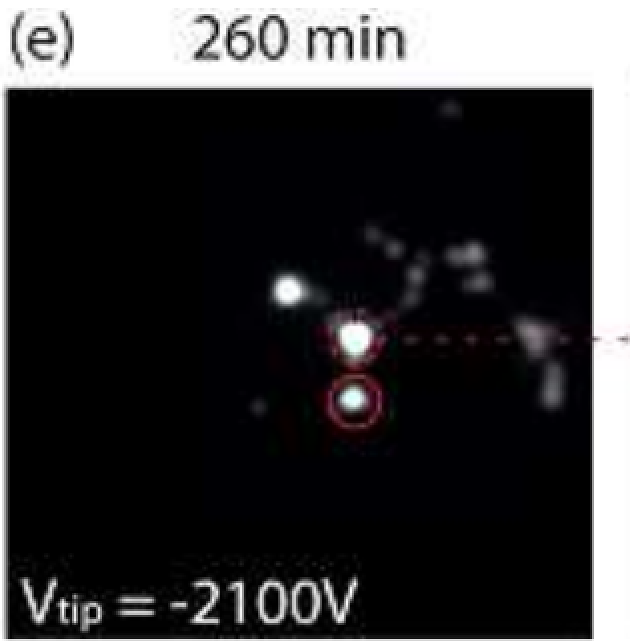
Ideal hemispherical surface emission pattern

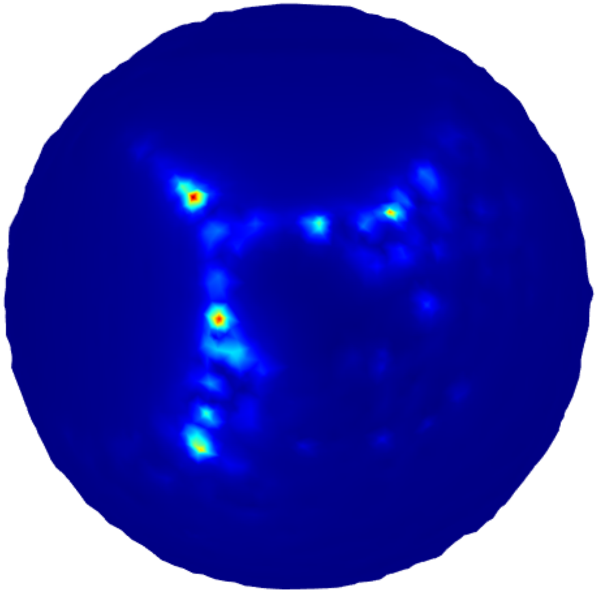


Hemispherical slightly relaxed MD surface emission pattern

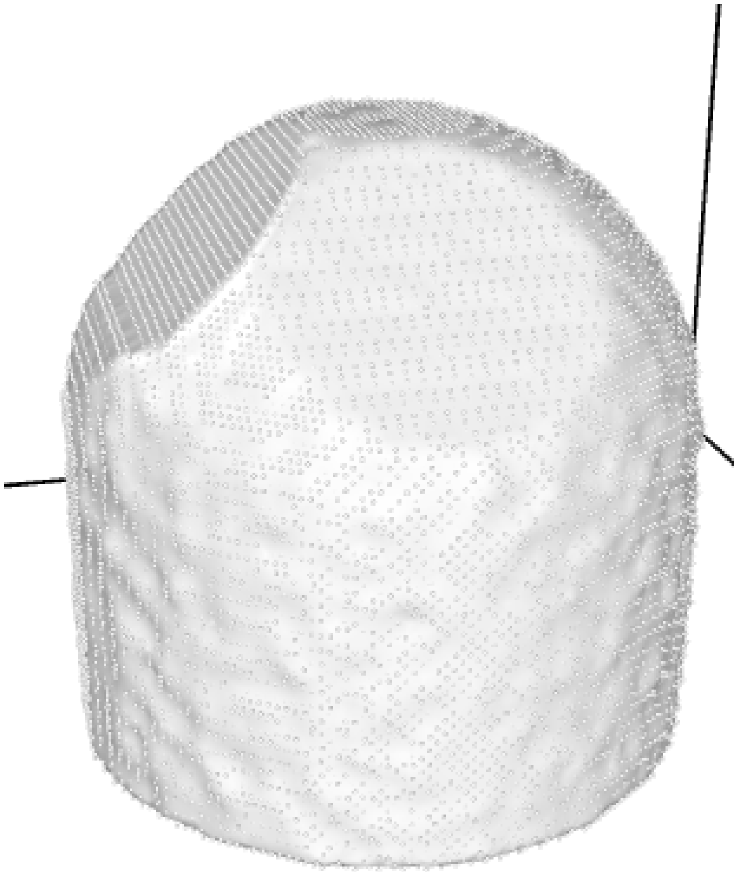
Emission patterns for atomistic surfaces





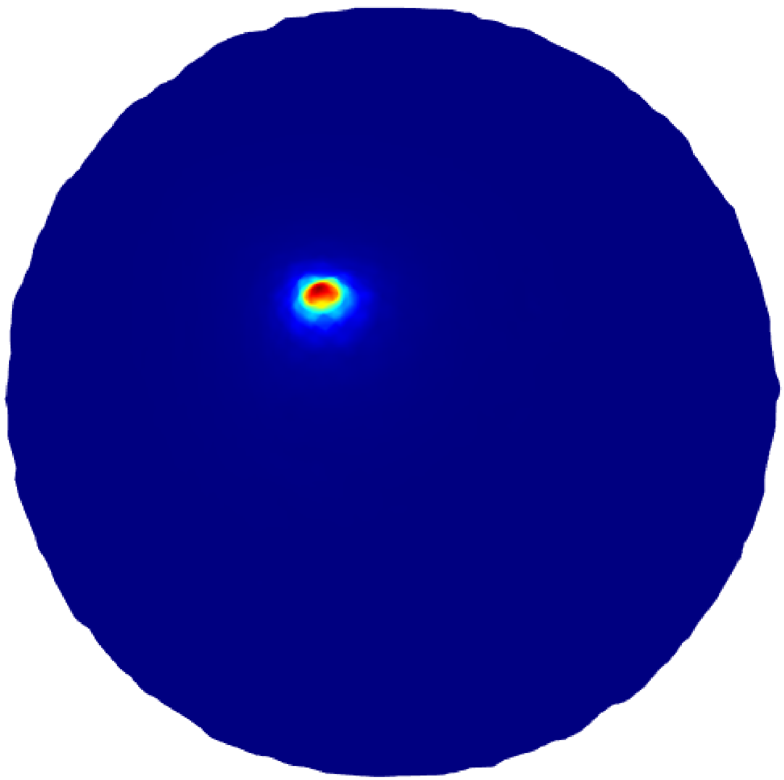


Emission pattern

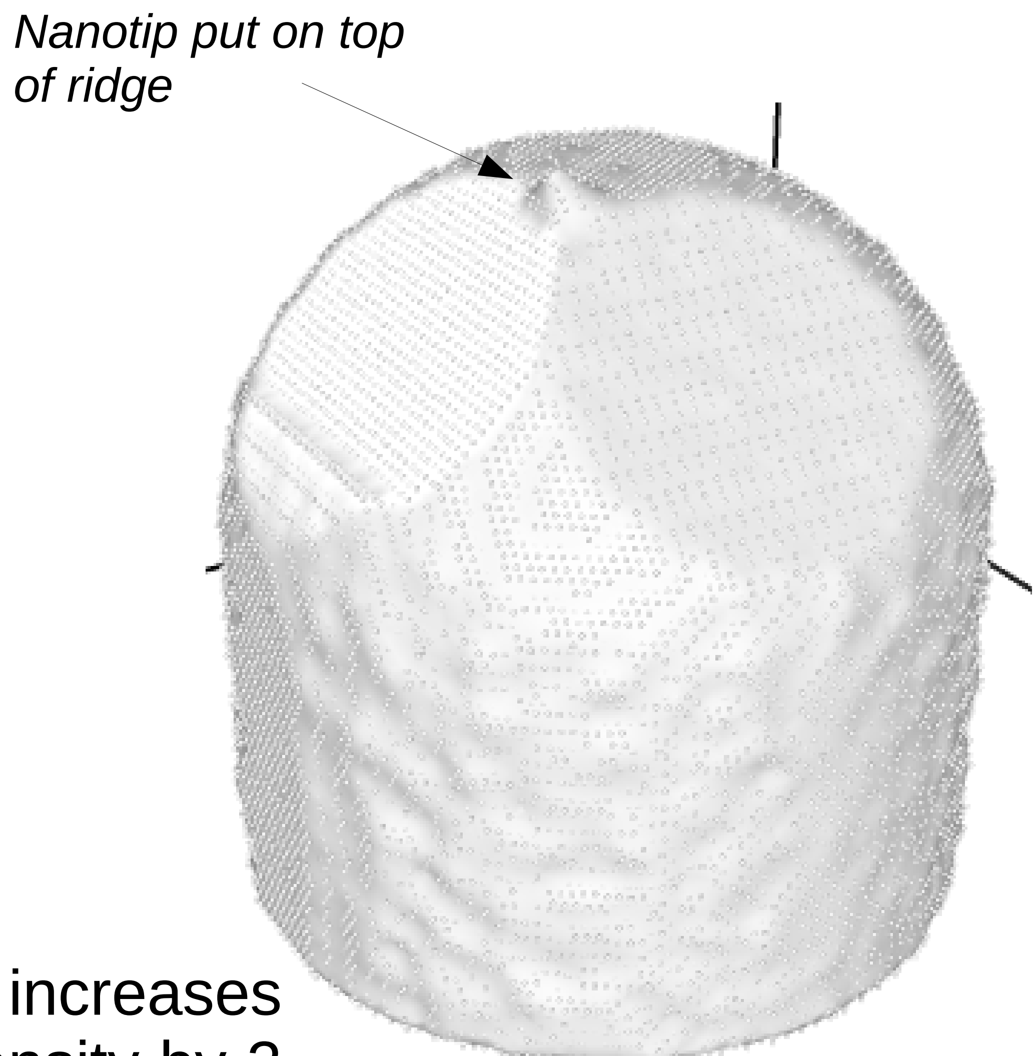


Atomistic tip, surface meshed

Emission patterns for atomistic surfaces

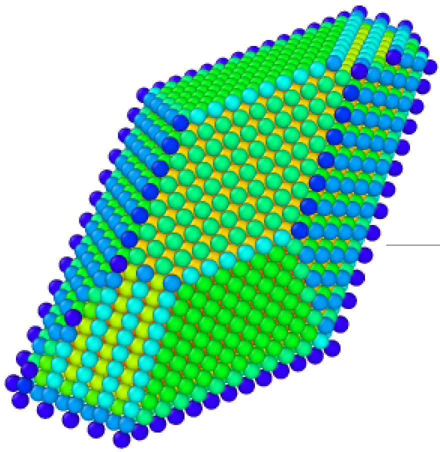


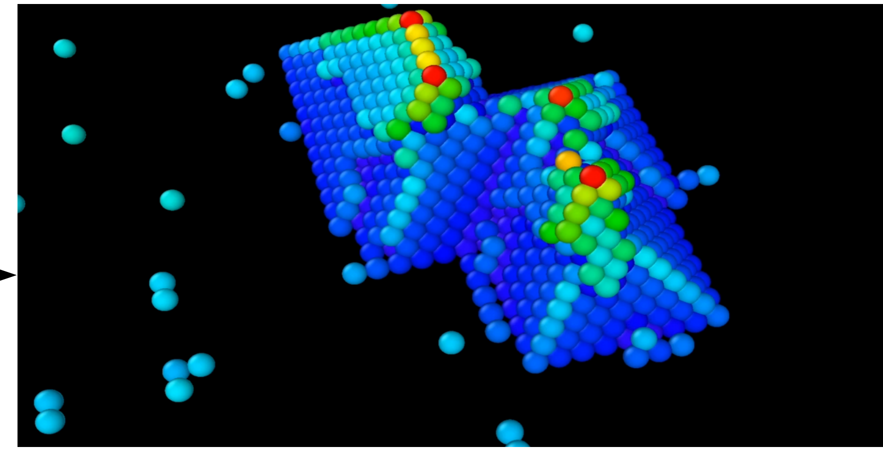
Emission pattern



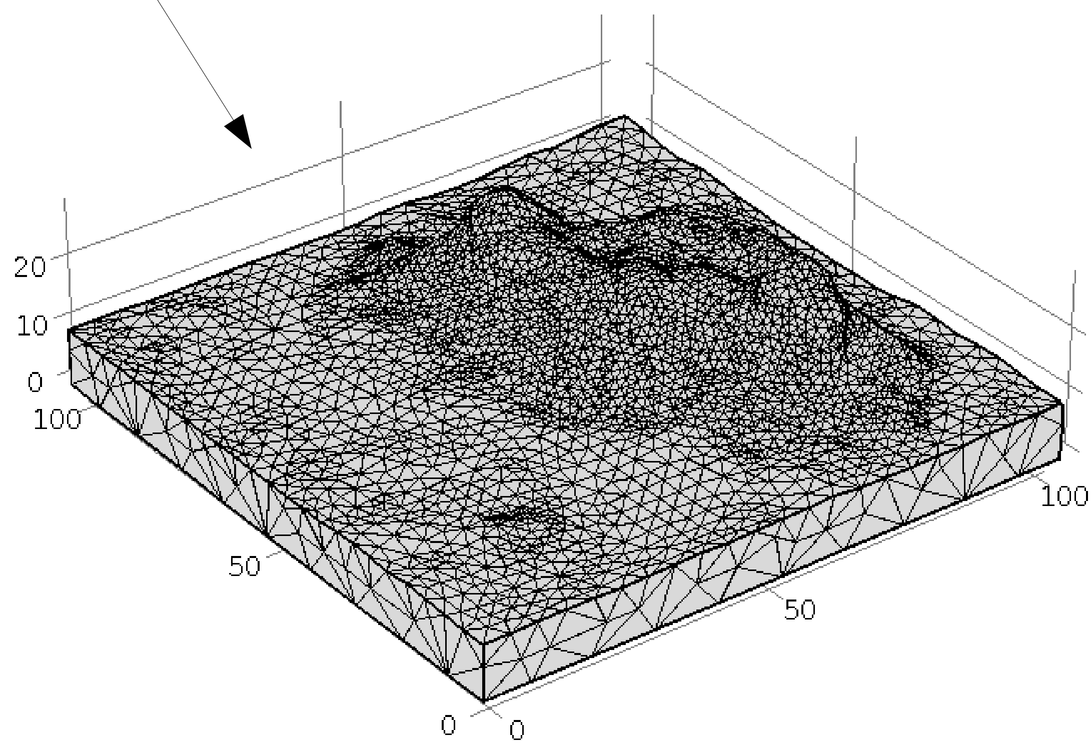
The presence of the nanotip increases maximum emission current density by 2 orders of magnitude

Diffusion affecting emission patterns

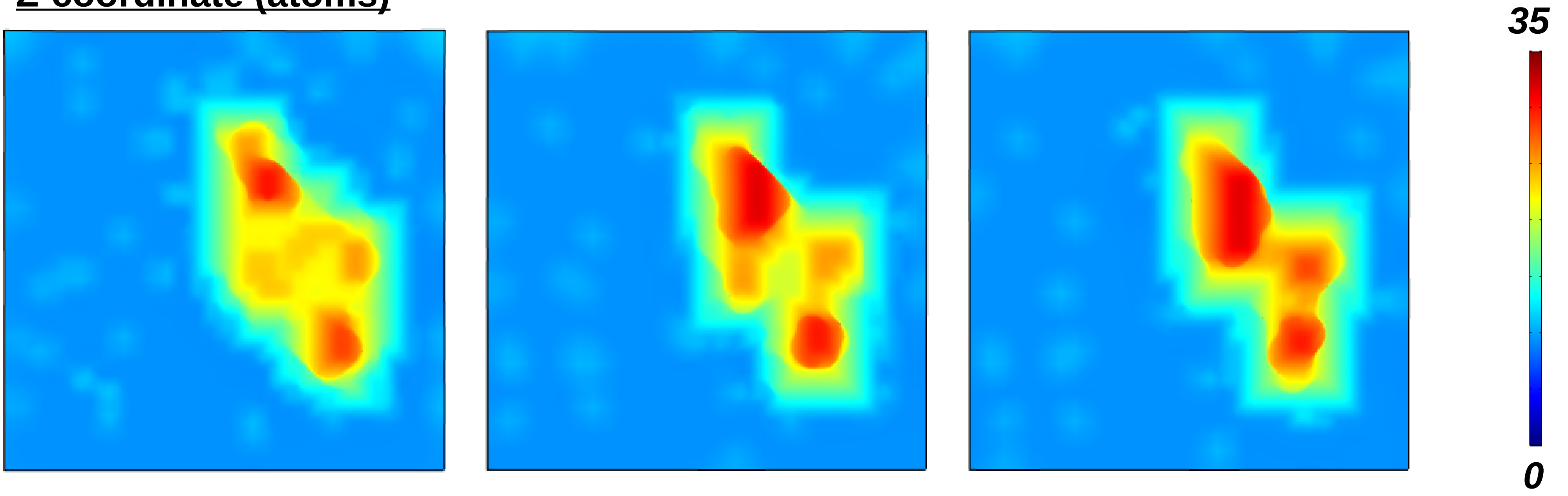




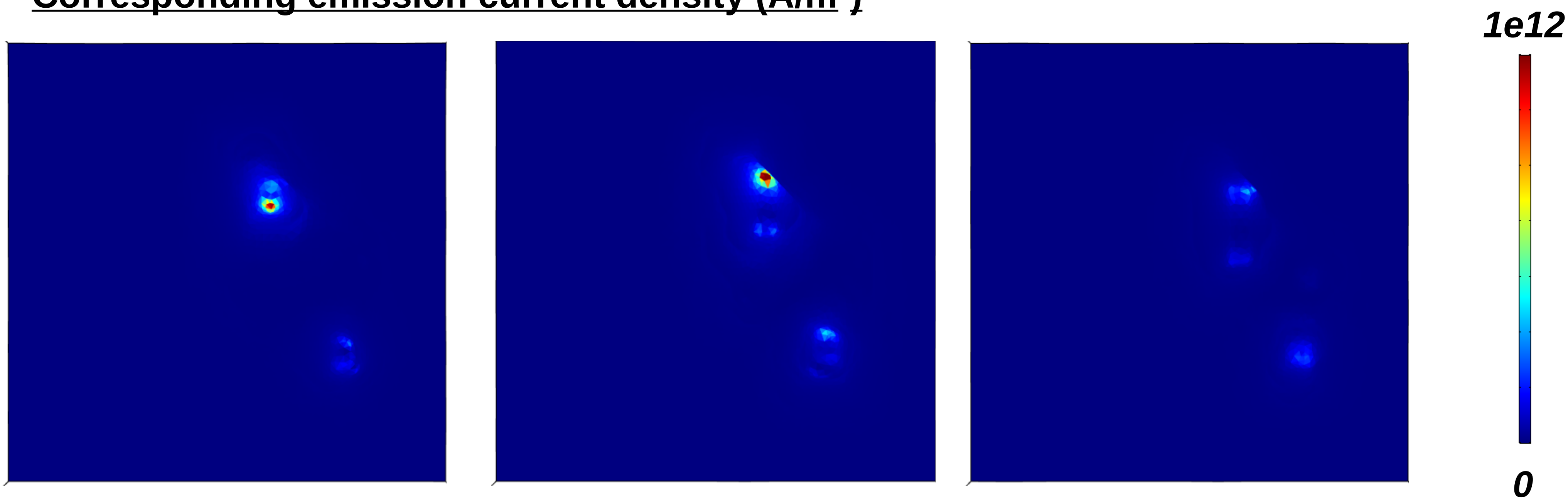
Using KMC with electric field at 2500 K and 0.5 GV/m, a plateau starts growing tip-like structures



Z-coordinate (atoms)



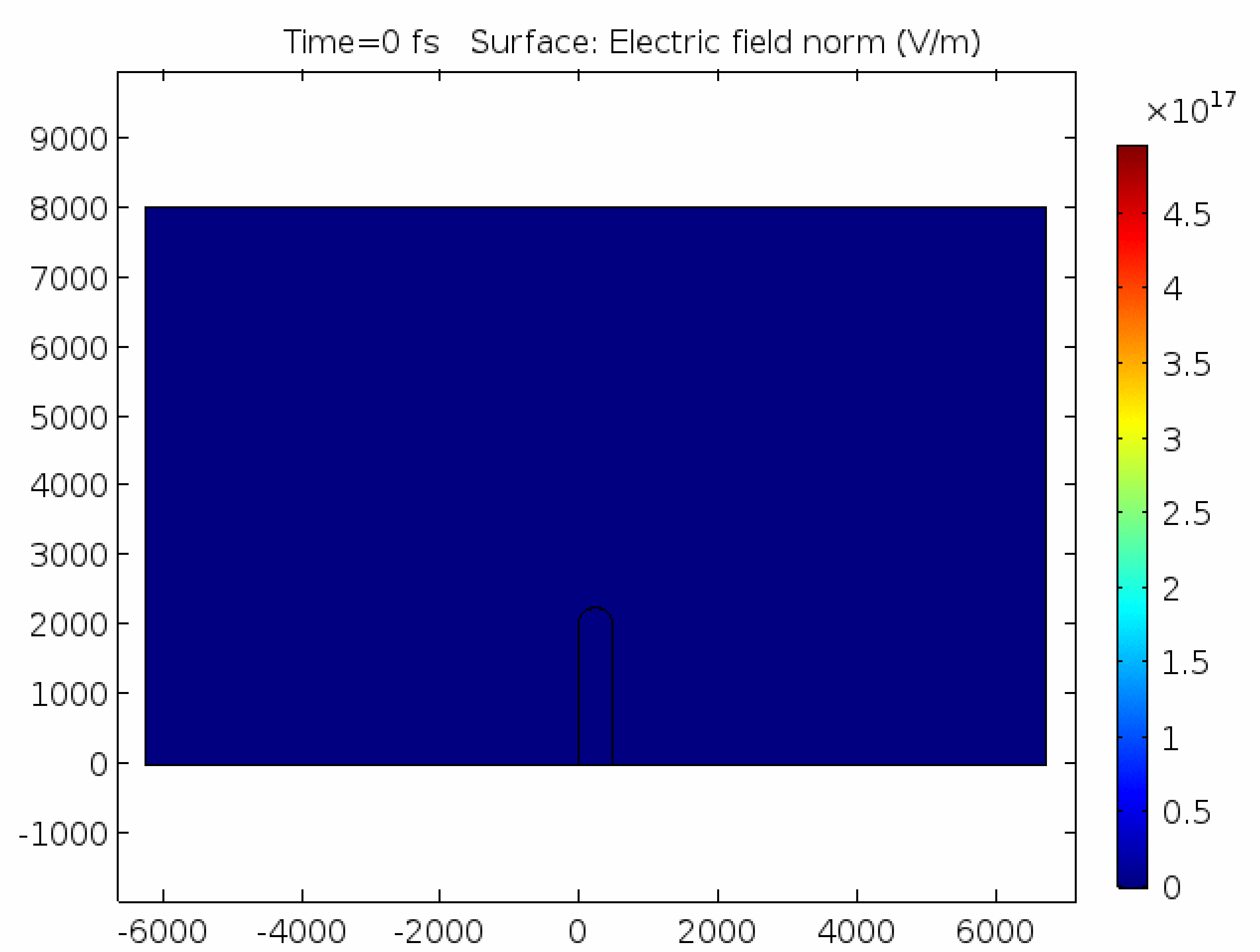
Corresponding emission current density (A/m^2)



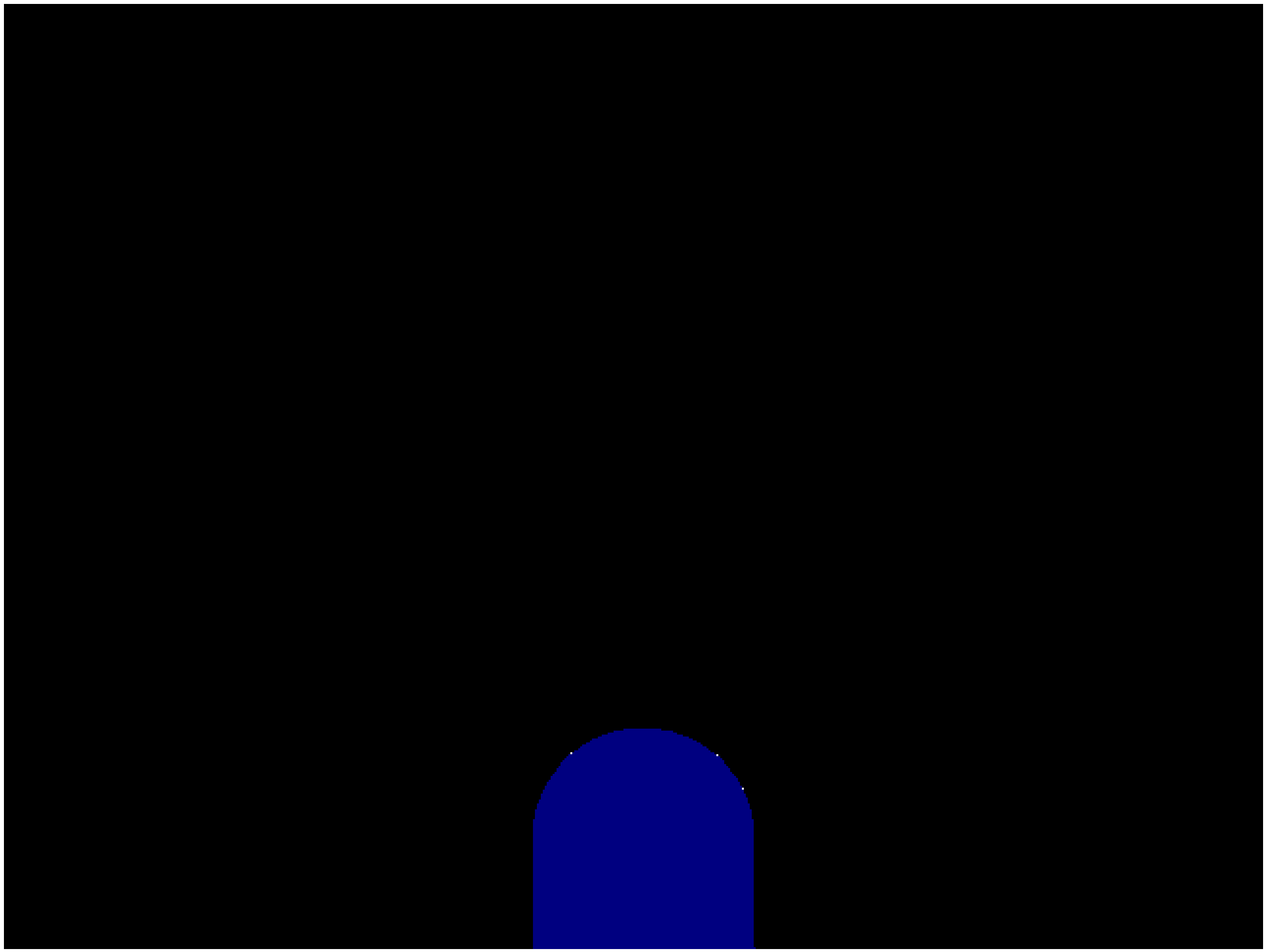
Chronological order of surface evolution

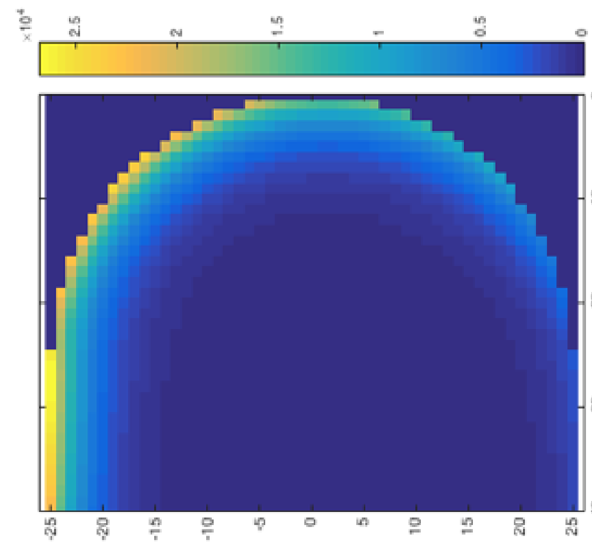
Ongoing work

- Laser beam modulation as EM-field, coupled with Tungsten crystal response
- Larger atomistic surfaces for longer periods



EF energy dissipation





Currently used energy deposition is static. In a laser impulse the EM-field modulation ensures that cannot be so.

Electric field norm in grayscale; Energy deposition in rainbow.

Conclusions

- Laser heating may be somewhat underestimated; surface melting cannot be ruled out.
- Laser energy deposition occurs in a very thin layer on the surface
- MD/KMC-FEM hybrid analysis shows that remarkably clear faceting is needed to reproduce topography-following emission patterns
- Difficult to analyze stress behaviour due to possible melting, but plastic thermal deformations should be possible