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Thermal, electrical and mechanical simulations of field emitters using Finite Element Method

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MEVARC 2015

Layout of the presentation

- What we simulate ….
- Brief overview of used models in FEM simulations
  - The emission currents and material heating
  - Mechanical stresses
- Multi scaling in FEM simulations
  - Atomistic surface reconstruction for continuum simulations
- First insights into mechanical stresses in kMC nanostructures

FEM simulations of field emitters

Comparison of simulation and experiment:
Emission current measurements

Electric field over surface:
Emission currents
Surface stress

- Surface stress due to high electric field
- Emission currents

Material Surface Simulations:
Field emitters
Surface reconstruction

- High aspect ratio tips
- Field emitters

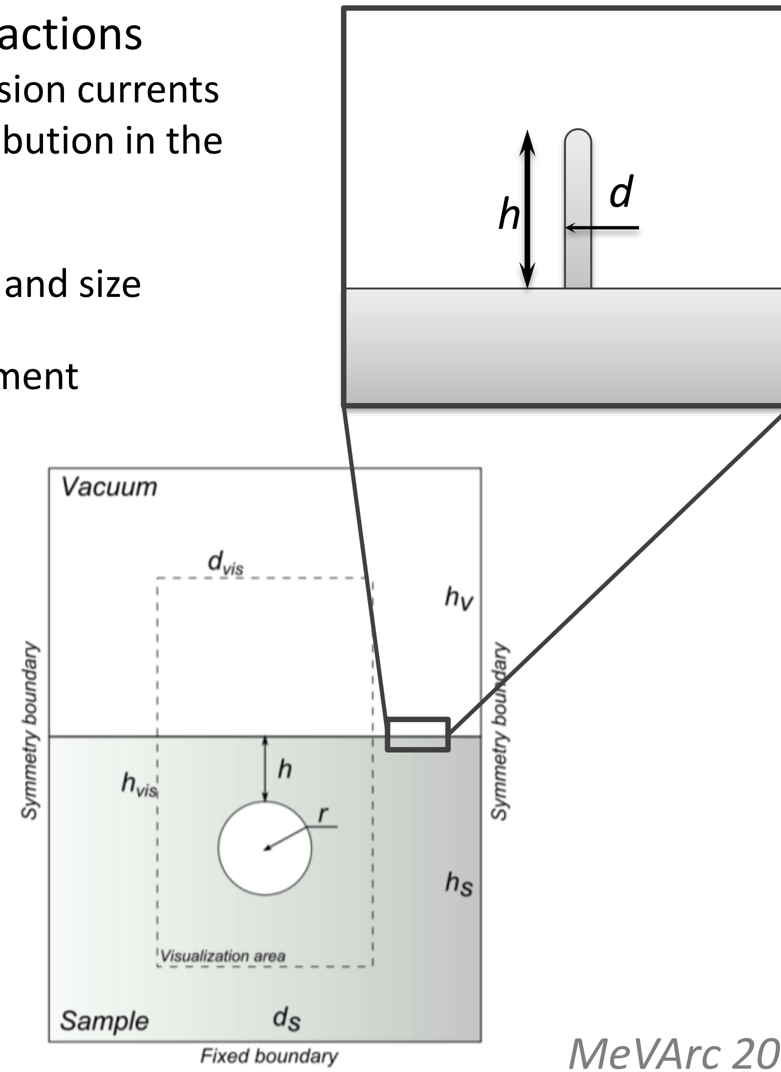
Bulk simulations:
Multiscaling, coupling to other methods
kMC, MD, FEM
Strongest/weakest nanostructure estimation

Subsurface voids, precipitates as stress concentrators

Dislocations and plastic deformation as source of emitters

Simulated systems

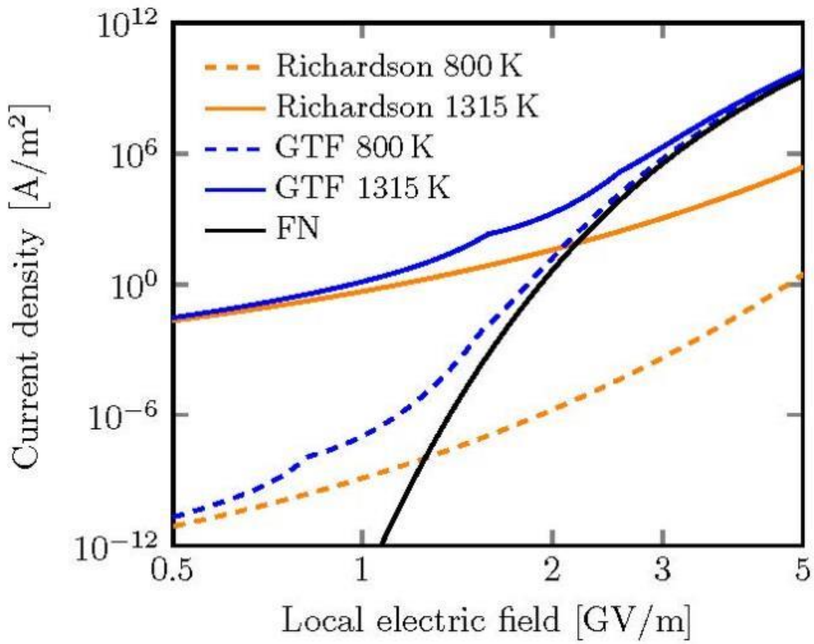
- Coupled electric, mechanical, thermal interactions
  - Electric field deforms sample and causes emission currents
  - Emission currents lead to current density distribution in the sample
  - Material heating due to the electric currents
  - Electric and thermal conductivity temperature and size dependent
  - (Deformed) sample causes local field enhancement



- Dc El. field ramped up to 14 000 MV/m
- Comsol Multiphysics 4.4 (and 5)
  - Nonlinear Structural Materials Module
  - AC/DC module
- HELMOD (Combined Electrodynamics, Molecular dynamics)
- LAMMPS
- Kimocs (by Ville Jansson)
- Simulated materials: Copper

The emission currents

General Thermal Field model - Simulations of emission currents over large surfaces



- Thermionic emission: high temperature, low field
- Field emission: low temperature, high field
- Combined effects : general thermal field equation:

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

$$N(n,s) \approx n^2 \Sigma\left(\frac{1}{n}\right) e^{-s} + \Sigma(n) e^{-ns},$$

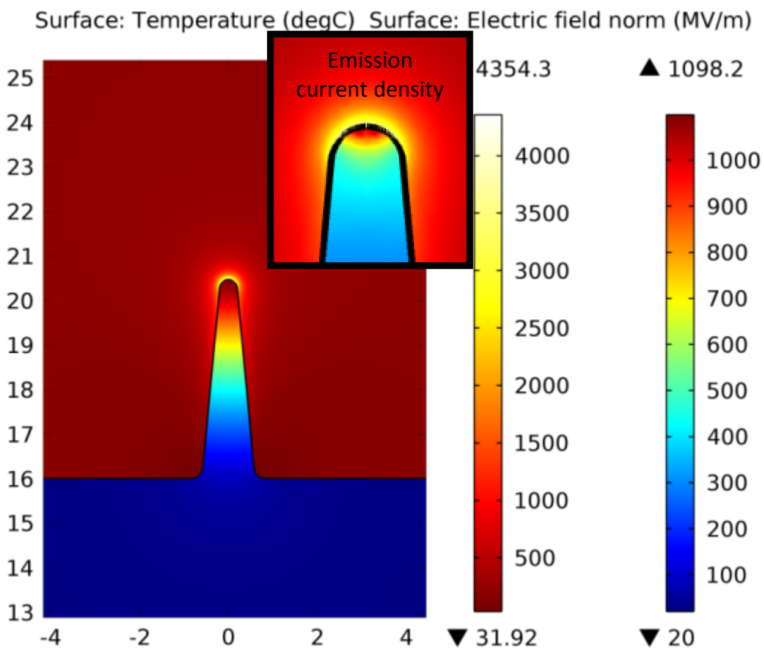
Special interest:
Intermediate region where thermal contribution can be significant

V. Zadin, University of Tartu

K. L. Jensen, J. Appl. Phys. (2007)

Heating and emission currents

Local emission currents – connection to the experiment



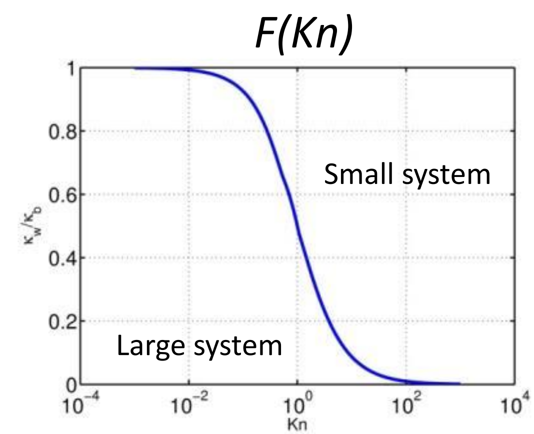
- Heat equation in steady state
- Fully coupled currents and temperature
- Emission currents concentrated to the top of the tip
- **Nottingham effect included in thermal modelling**

Field emitters as nanowires

$$\sigma_w = F(Kn)\cdot\sigma_b$$

$$\kappa_w = F(Kn)\cdot\kappa_b$$

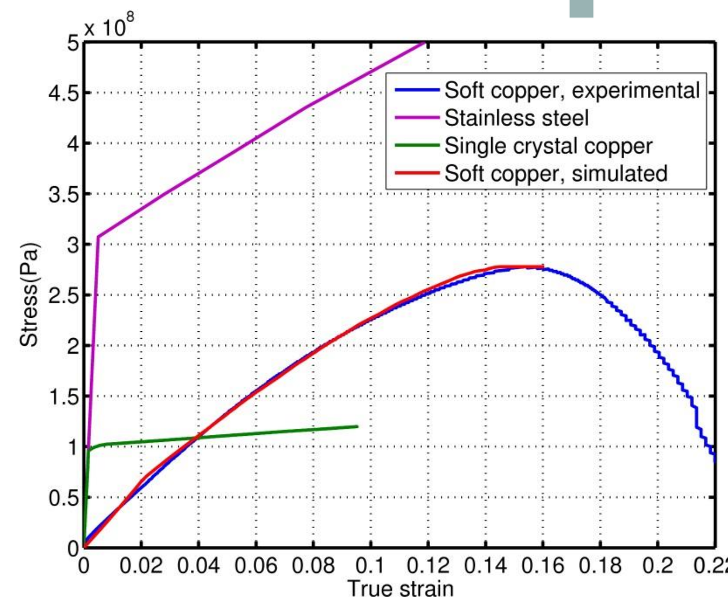
$$Kn = \frac{L_{free}}{d}$$

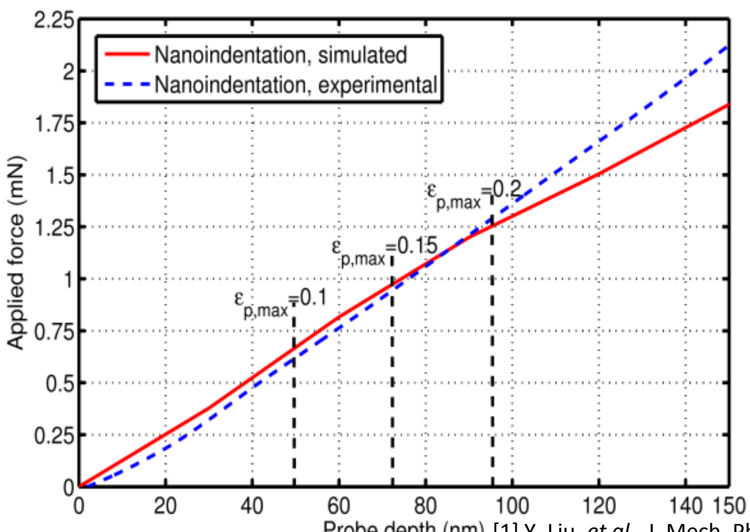


- Size dependence of electric and thermal conductivity
- Conductivity in nanoscale emitters is significantly decreased (more than 10x for sub-nanometer tip)
- Knudsen number to characterizes nanoscale size effects
- Wiedemann-Franz law for thermal conductivity
- **Optionally, temperature dependence in finite size effects**

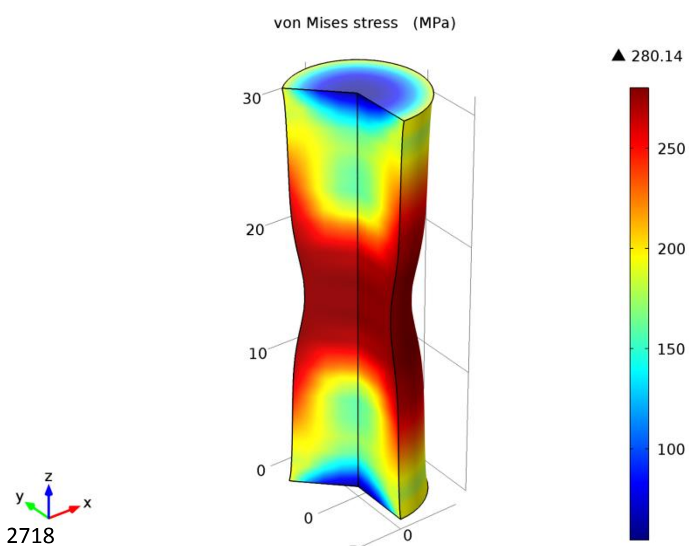
Elastoplastic deformation simulations

- Elastoplastic deformation of material, simulation of large strains
- Validation of material model and parameters by conducting tensile stress simulations
- Accurate duplication of the experimental results (tensile and nanoindentation test)
- **Parameters from tensile test are macroscopic, single crystal parameters are needed due to large grains in soft copper**
- **Incorporation of surface effects to anisotropic elastic material model in progress**



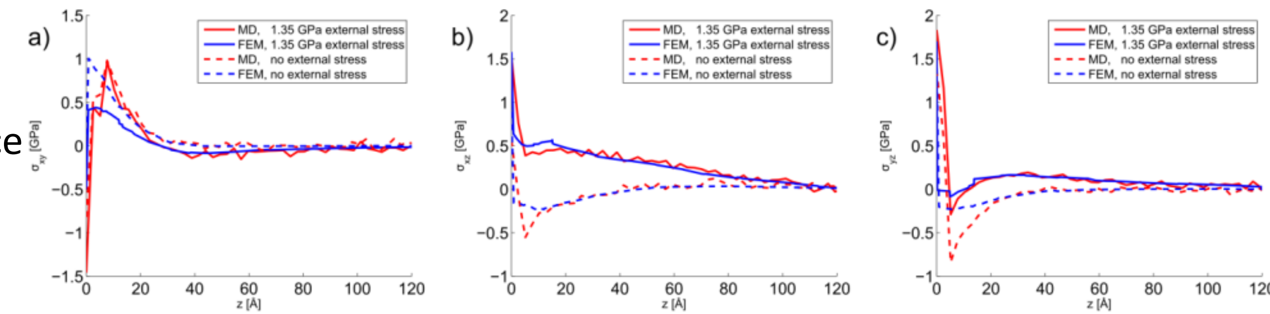


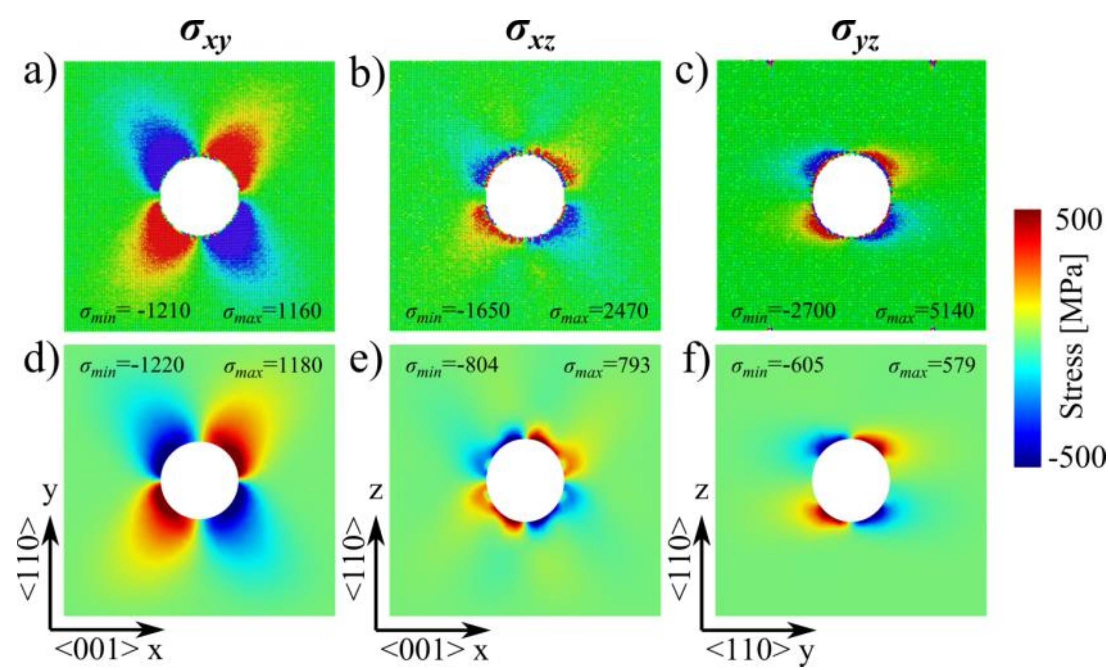
[1] Y. Liu, *et al.* ,J. Mech. Phys. Solids, 53 (2005) 2718



Surface stress effects in nanoscale modelling

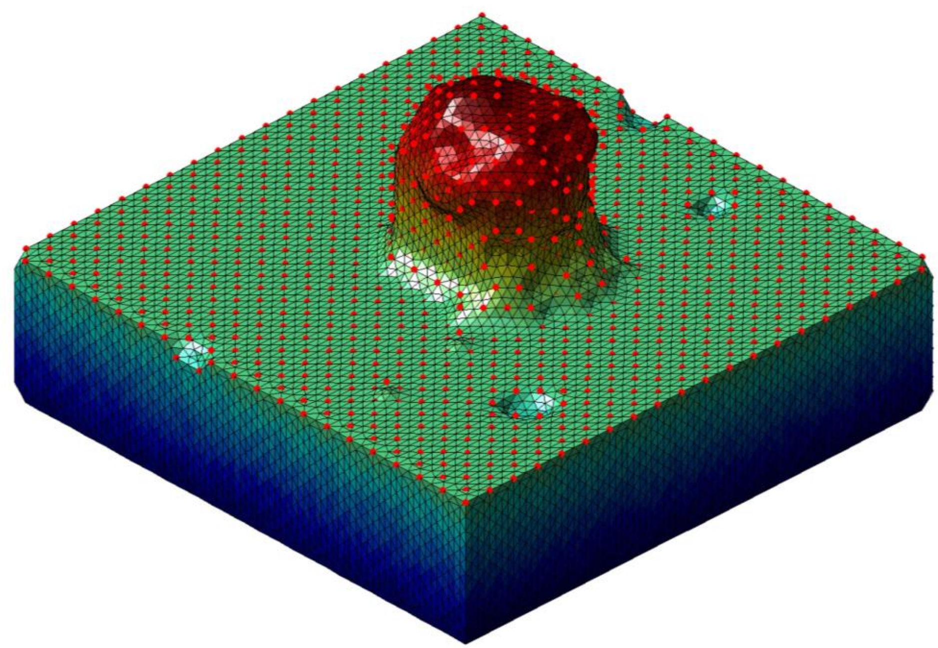
- Anisotropic material model
- Crystal plane dependent surface properties
- The surface effects important below ~ 6-10 nm
  - Corrections for surface stress (surface tension)
  - Model complexity improved towards nonlocal simulations
  - Strongest/weakest nanostructure estimation
- Plastic deformation
  - Accurate limits to be determined
  - Dependence from grain size, average dislocation length and plastic deformation activation volume
  - More complex model needed to account microstructure effects, dislocation densities etc.





Surface reconstruction based on kMC simulations

- Surface reconstruction from KMC simulations
  - Material stress calculations
  - Temperature and emission currents estimation
- Delaunay triangulation
  - No atoms in the circumcircle of a tetrahedra
    - Coarse mesh – maximum edge length is lattice_constant
    - **Refined mesh – maximum edge length is lattice_constant/2**
- Influence of sharp corners is controlled using Laplacian smoothing of refined mesh

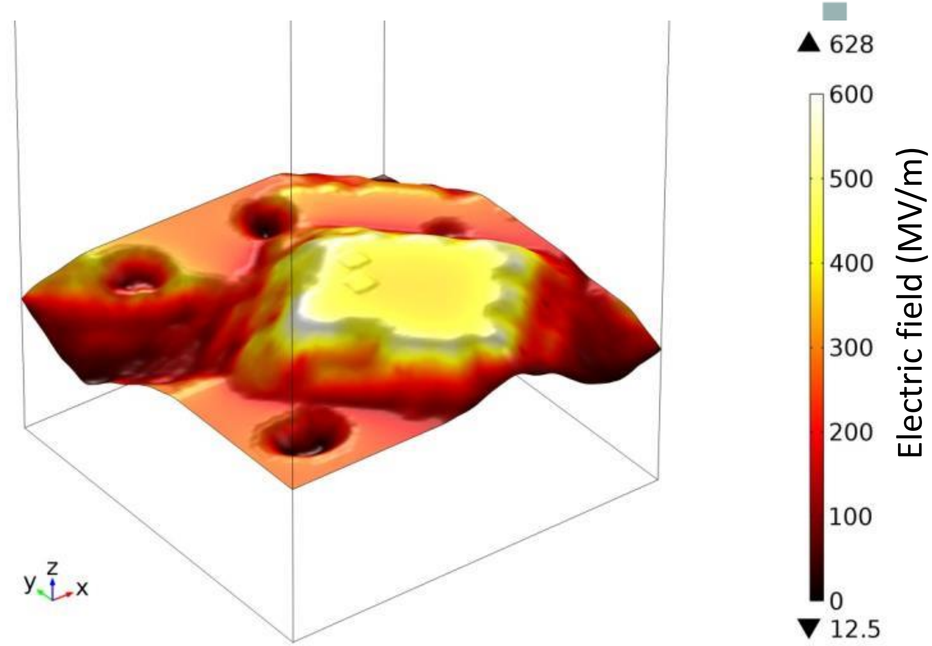


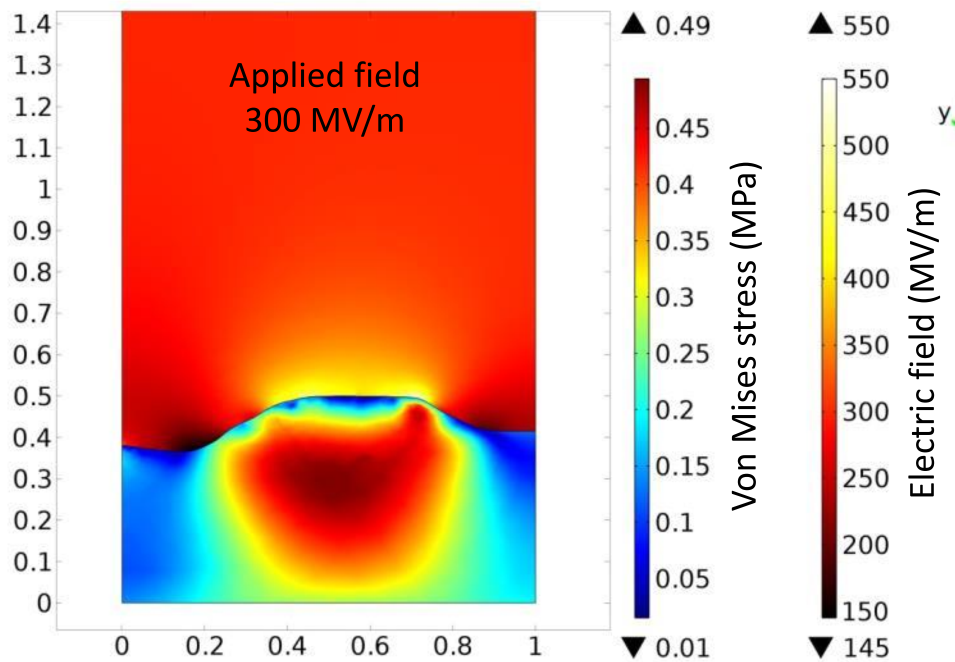
Methodology is not limited to KMC

Future MD or experimental surface reconstruction is possible

El. field and stress distributions

- Included physics:
  - Electric field and electrostatic stress
  - Material stress (surface stress not yet included)
  - Emission currents (GTF) and temperature
- One way coupling – Kimocs to FEM

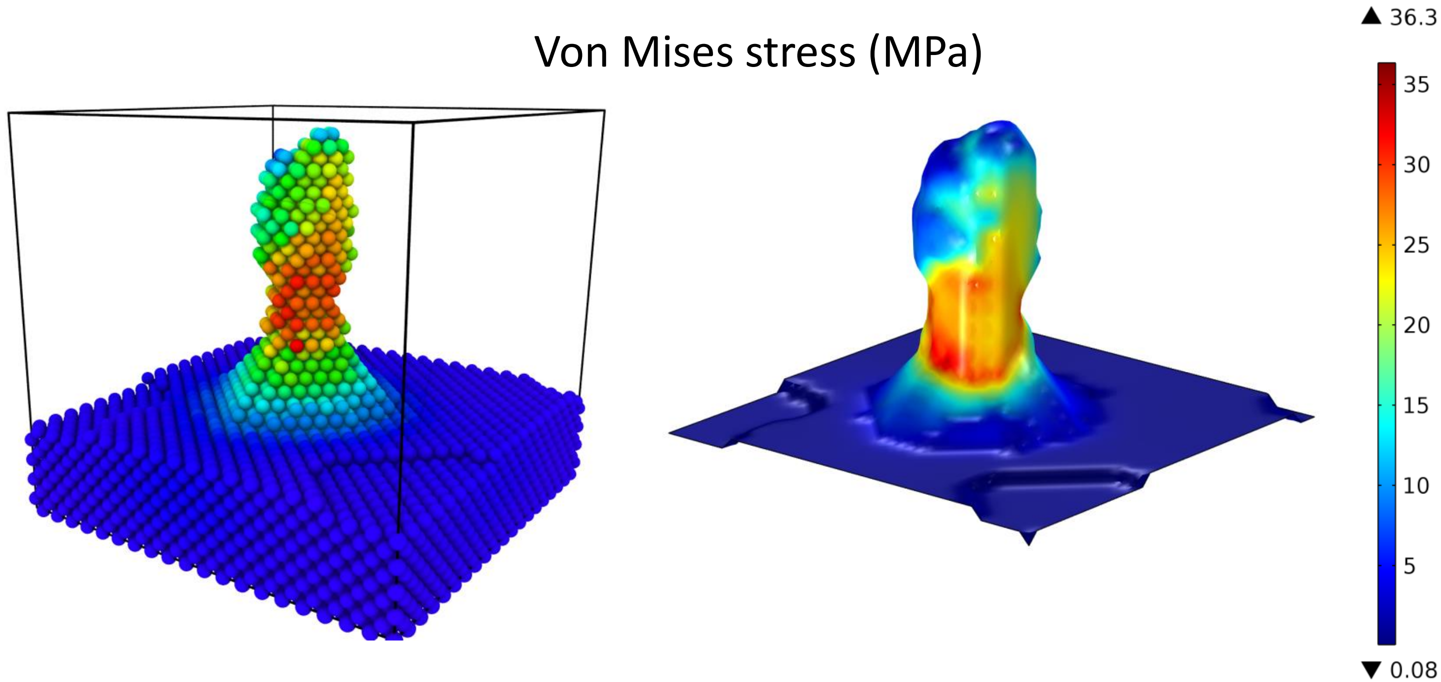




From FEM simulations:

- Interpolation in atom locations:
  - Mechanical stress
  - Current density
  - Material temperature

Simulation outputs



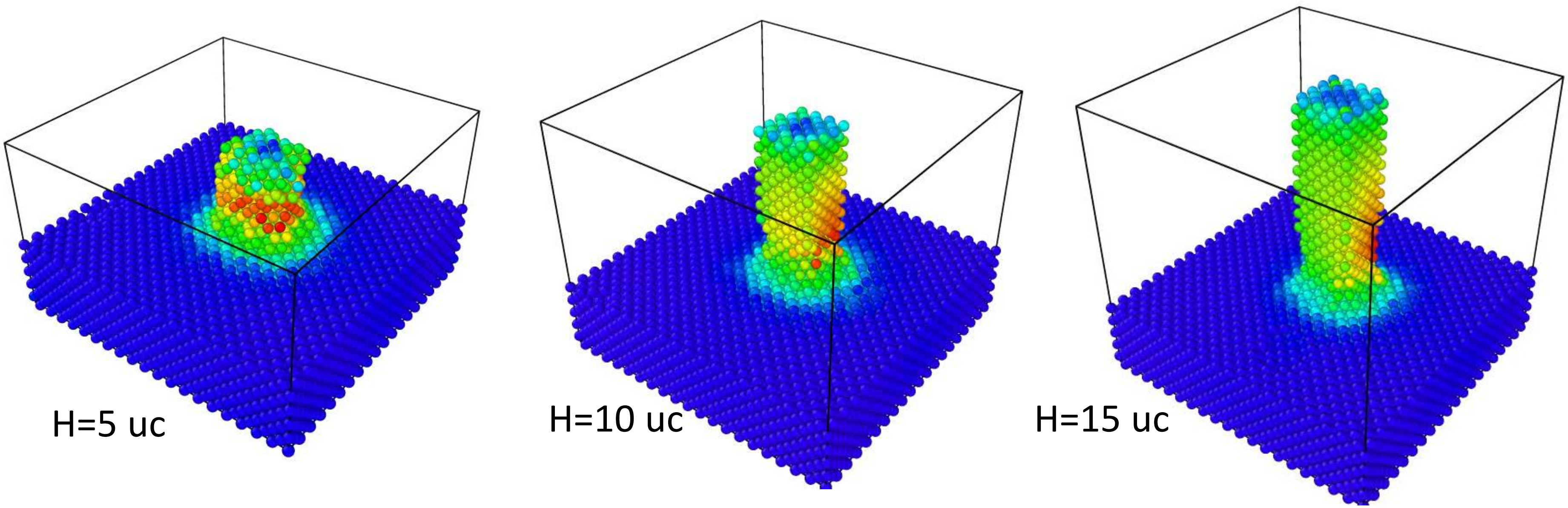
The Good:

- Robust surface detection – all geometries and surfaces can be handled
- All our existing FEM models can be used

The Bad:

- Influence of adatoms needs better handling
- Emission currents from ultra small areas – single atom can emitter most of the current
- Speed optimization needed!

Stress in field emitters



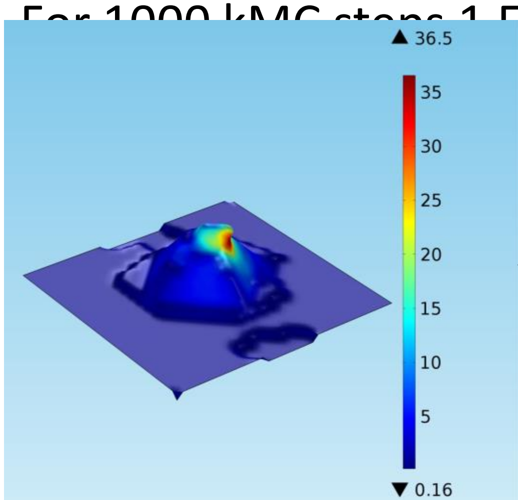
- Reasonable behavior of stress assigned to atoms
  - The link between methods working
- Nonuniform and complex stress distribution
  - Can lead to additional deformation of the sample

Further points of interest:

- The effect of mechanical stress
- **The influence of dynamic geometry to the emission currents and field enhancement**
- Thermal stability of the emitter

El. field and stress evolution

- For 1000 kMC steps 1 FEM



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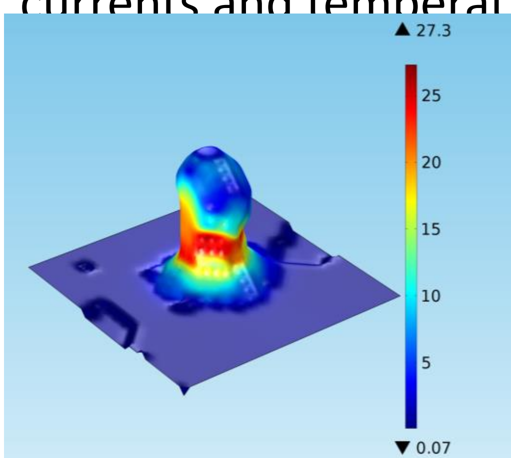
- Influence to the emission currents and temperature



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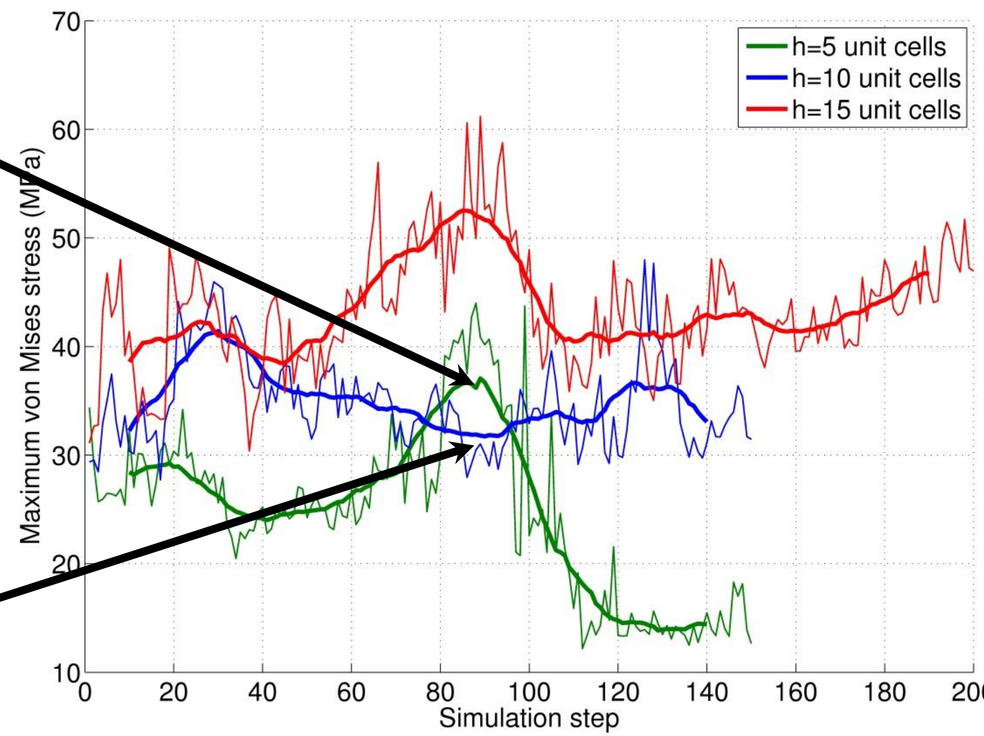
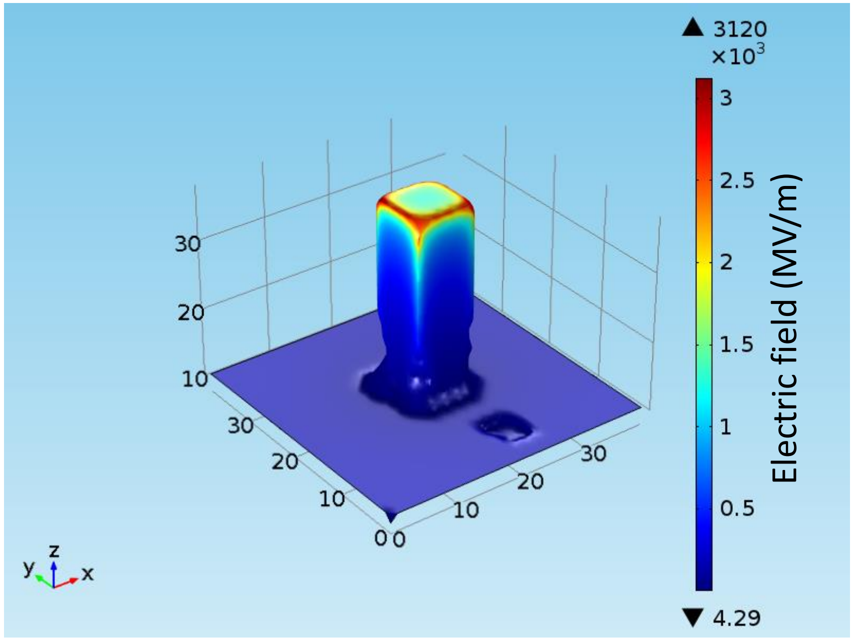


Bold lines – moving average

Emission current distribution mapping

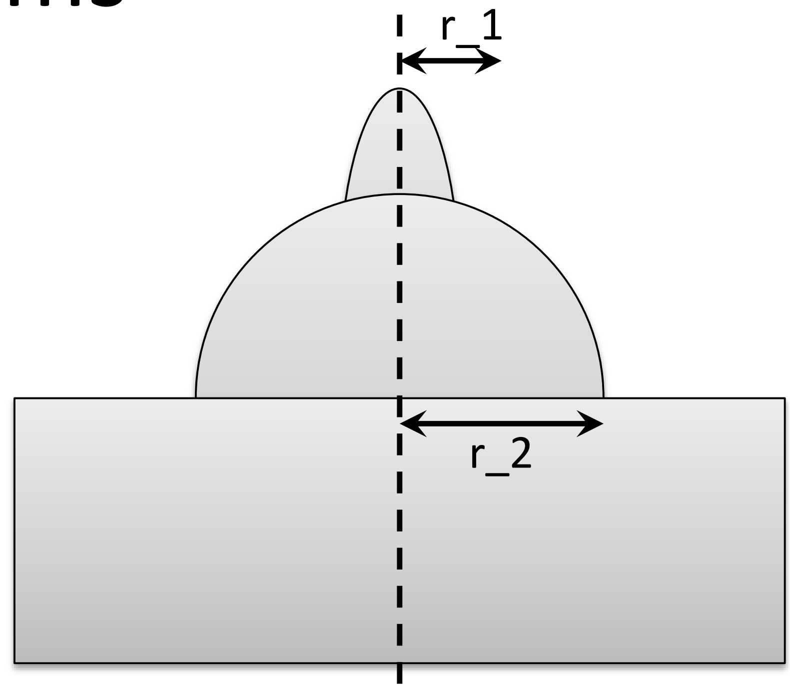
- El. field is not included in kMC simulation
- Edges of the protrusion have significant field enhancement
  - Possibilities for further enhancement due to Schottky conjecture
- Single atom can have significant influence over the emission currents
  - Additional homogenization is needed to reduce the effect
- **Points of interest:**
  - Evaporation mechanism in kMC
  - **Possible conditioning effect due to evaporation of sharp corners?**



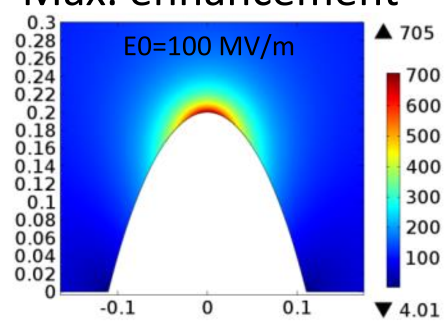
Model for emission currents needs updating to include curvature effects

Sensitivity to surface perturbation – influence of adatoms

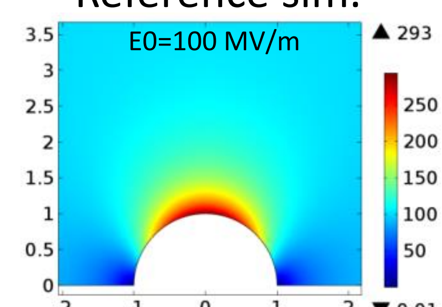
- We can see different surface modifications leading to small β
  - Large β is needed
- Multiplication of field enhancement factors
  - Can explain observed high beta values
- Incorporates surface roughness
- r_1/r_2<0.1 is needed to observe significant influence



Max. enhancement



Reference sim.



Conclusions

- FEM is viable and flexible tool for studying surface modification phenomena
- Important to improve the accuracy of emission current modeling
  - Curvature effects must be included
- Future simulations of possible conditioning mechanisms – evaporation of “hot” atoms

Thank you for your attention!