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Electro-mechanical and thermal simulations of surface under electric field

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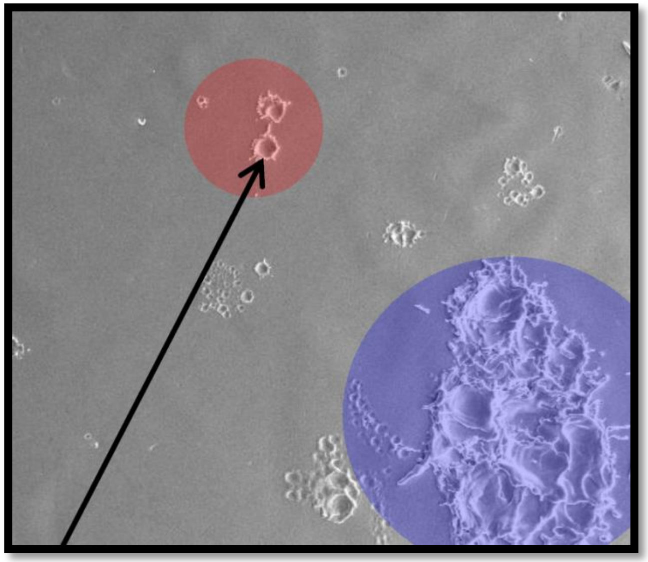
2013

Electrical breakdowns

Electrical breakdowns at CLIC accelerator accelerating structure materials

Accelerating el. field 100-150 MV/m

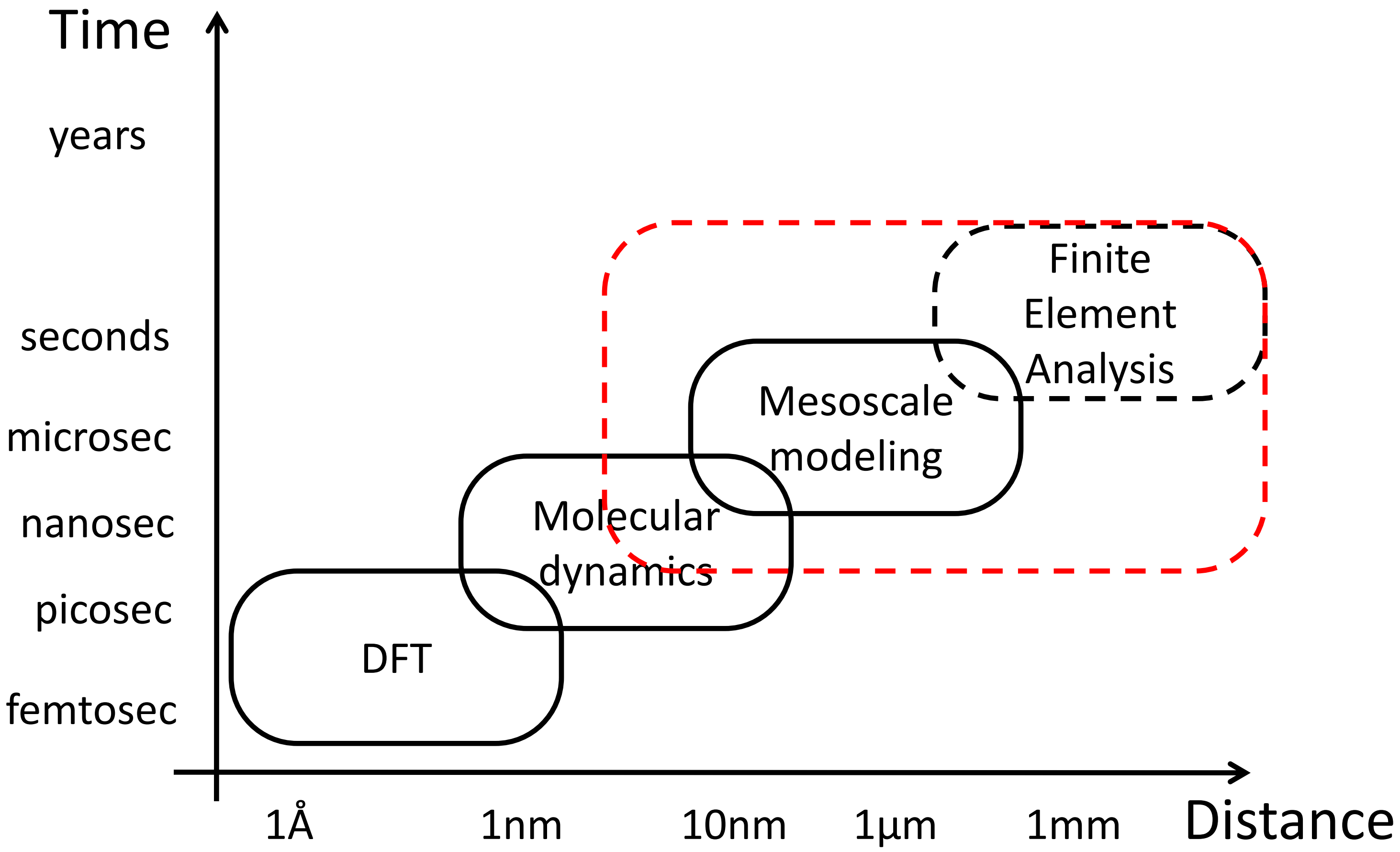
- Accelerating structure damage due to electrical breakdowns
- Local field enhancement up to factor 100
- Field enhancement caused by „invisible needles“



M. Aicheler, MeVArc 2011

Electrical breakdown rate must be decreased under $3 \cdot 10^{-7}$ 1/pulse/m

Computer simulations in Chemistry and Physics



Time

years

seconds

microsec

nanosec

picosec

femtosec

DFT

Molecular dynamics

Mesoscale modeling

Finite Element Analysis

1Å

1nm

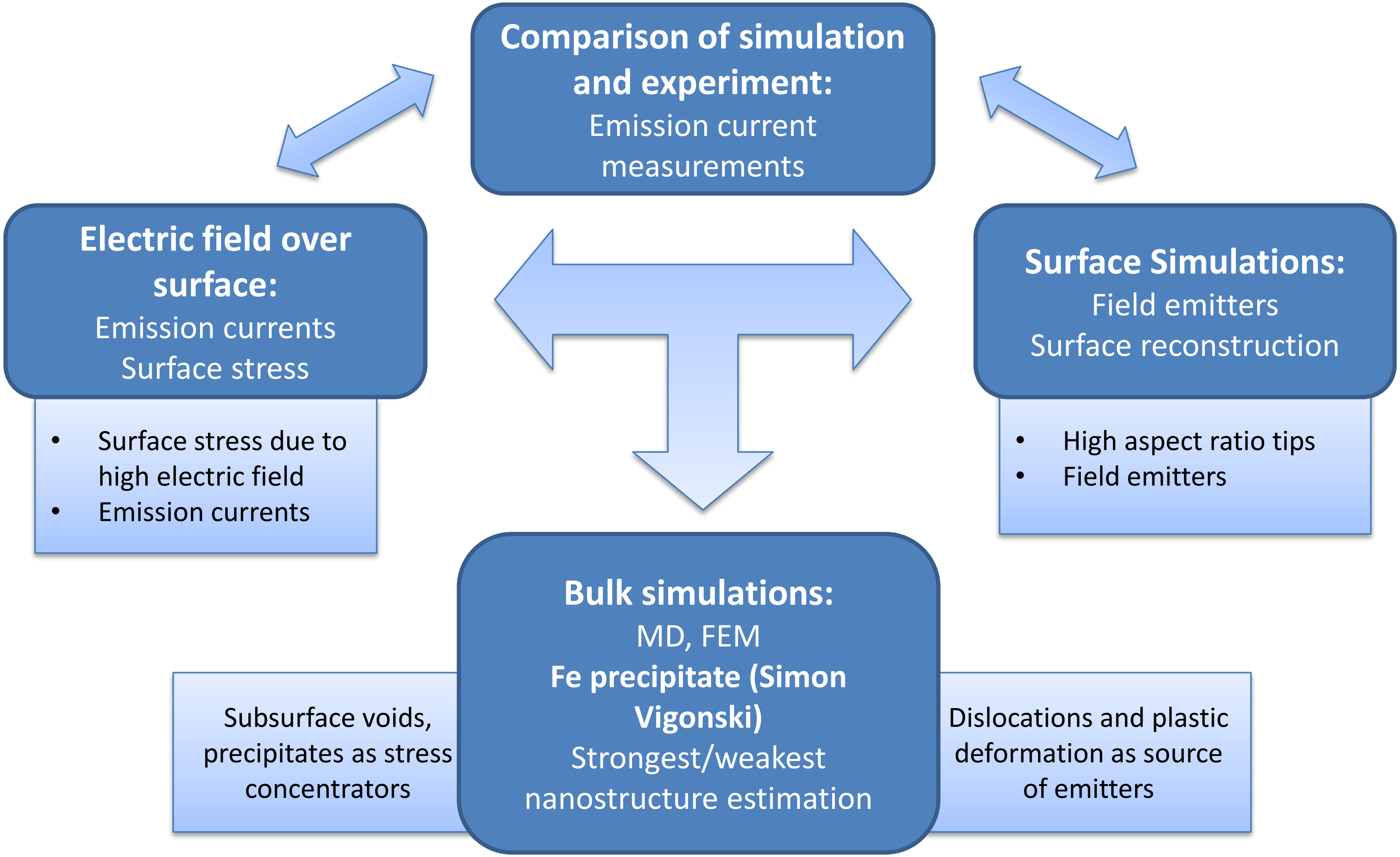
10nm

1µm

1mm

Distance

The simulations of surface and bulk



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

Surface Simulations:
Field emitters
Surface reconstruction

- High aspect ratio tips
- Field emitters

Bulk simulations:
MD, FEM
Fe precipitate (Simon Vigonski)
Strongest/weakest nanostructure estimation

Subsurface voids, precipitates as stress concentrators

Dislocations and plastic deformation as source of emitters

The stress concentrators

- The void as source of dislocations
  - Void in material as stress concentrators
    - Spherical voids due to surface energy minimization
    - Single void in metal
  - Several mechanisms acting at once to produce the tip?
  - Understanding protrusion growth mechanism in the case of spherical void in DC electrical field
- Precipitates as stress concentrators (Fe)

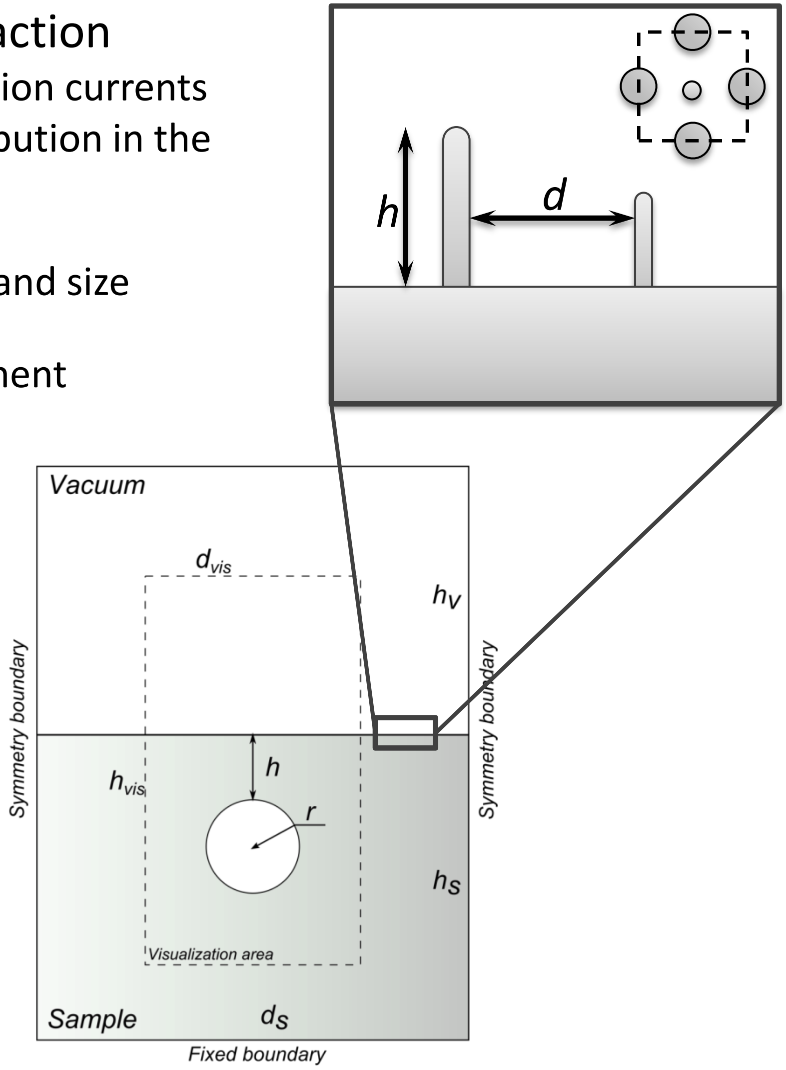
- High aspect ratio field emitters as initiators of a breakdown
  - Thermal and electrical behavior of field emitters
  - Mechanical behavior of field emitters

Current state of the model

- Complete description of the breakdown requires combination of several phenomenon
    - Mechanical response of the material
        - Elastoplastic material model
            - Anisotropic material with surface stress model
    - Applied electric field
    - Emission currents
        - Fowler-Nordheim equation
        - (Generalized thermal field and Nottingham effect - future)
    - Electric currents in the material and material heating
    - Deformable geometries
    - (Density of neutrals near surface - future)

Simulated systems

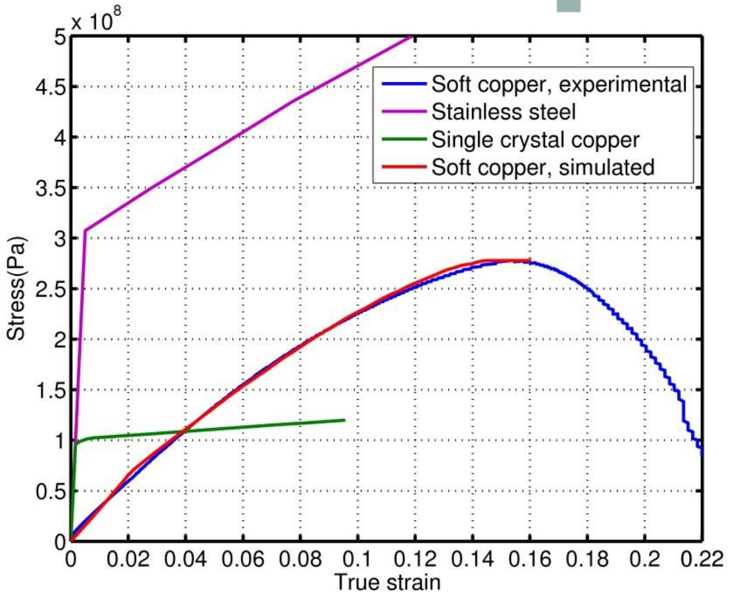
- Coupled electric, mechanical, thermal interaction
  - Electric field deforms sample and causes emission currents
  - Emission currents lead to current density distribution in the sample
  - Material heating due to the electric currents
  - Electric and thermal conductivity temperature and size dependent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



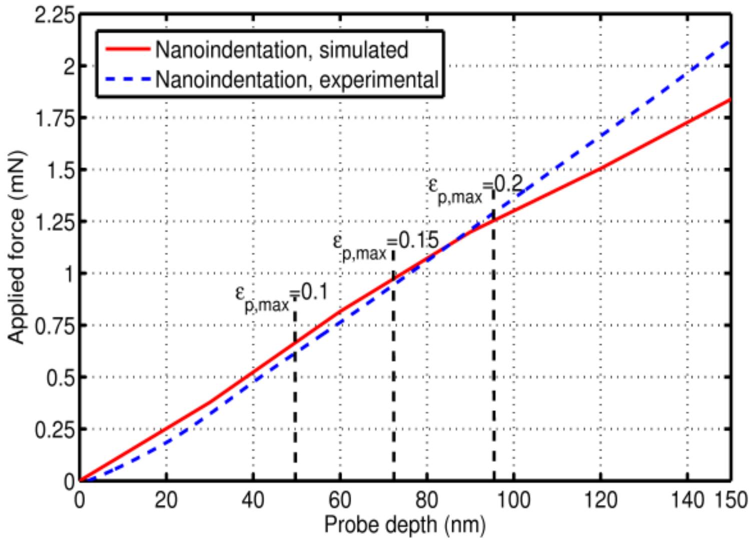
- Dc El. field ramped up to 10 000 MV/m
- Comsol Multiphysics 4.3b
  - Nonlinear Structural Materials Module
  - AC/DC module
- Simulated materials:
  - Soft copper
  - Single crystal copper
  - Stainless steel

Material model

- 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**



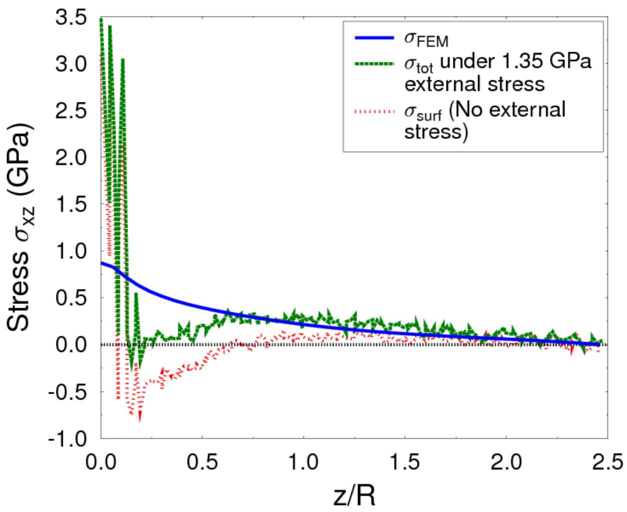
	Structural Steel	Soft Copper (CERN)	Single crystal copper [1]	Often used copper parameters
Young's modulus	200 GPa	3.05 GPa	57 GPa	110 GPa
Initial yield stress	290 MPa	68 MPa	98 MPa	70 MPa

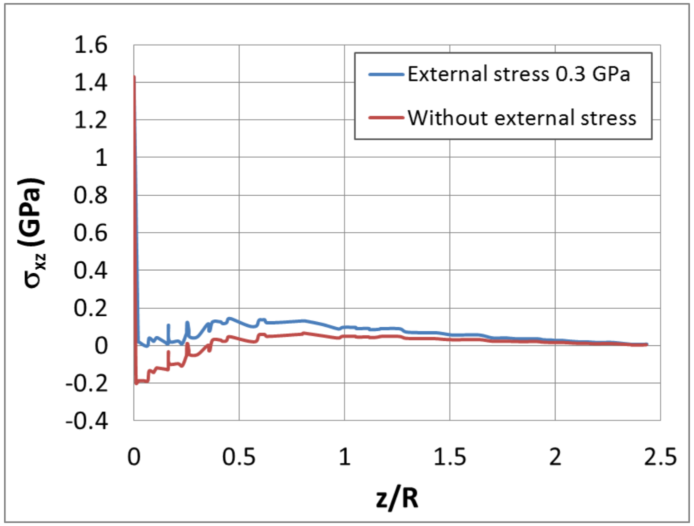


[1] Y. Liu, B. Wang, M. Yoshino, S. Roy, H. Lu, R. Komanduri,J. Mech. Phys. Solids, 53 (2005) 2718

The surface stress model – from MD to FEM to experiment

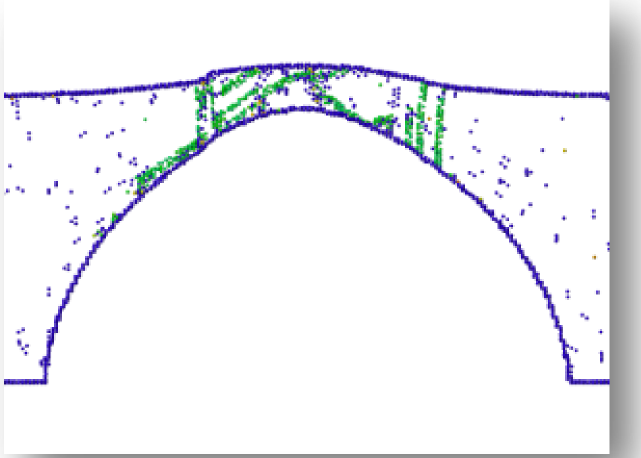
- Good scaling for linear elasticity
- Anisotropic material model
- Crystal plane dependent surface properties
- The surface effects important below ~ 6-10 nm
  - Corrections for surface stress (surface tension)
  - Model complexity improved towards nonlocal simulations
  - Strongest/weakest nanostructure 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.

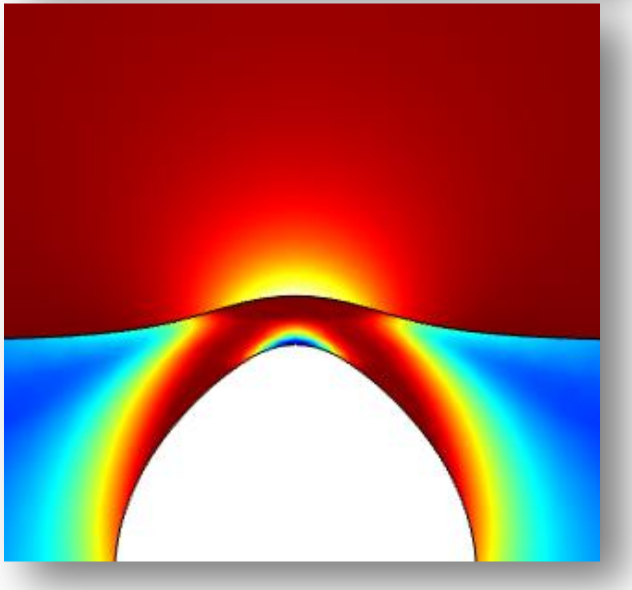




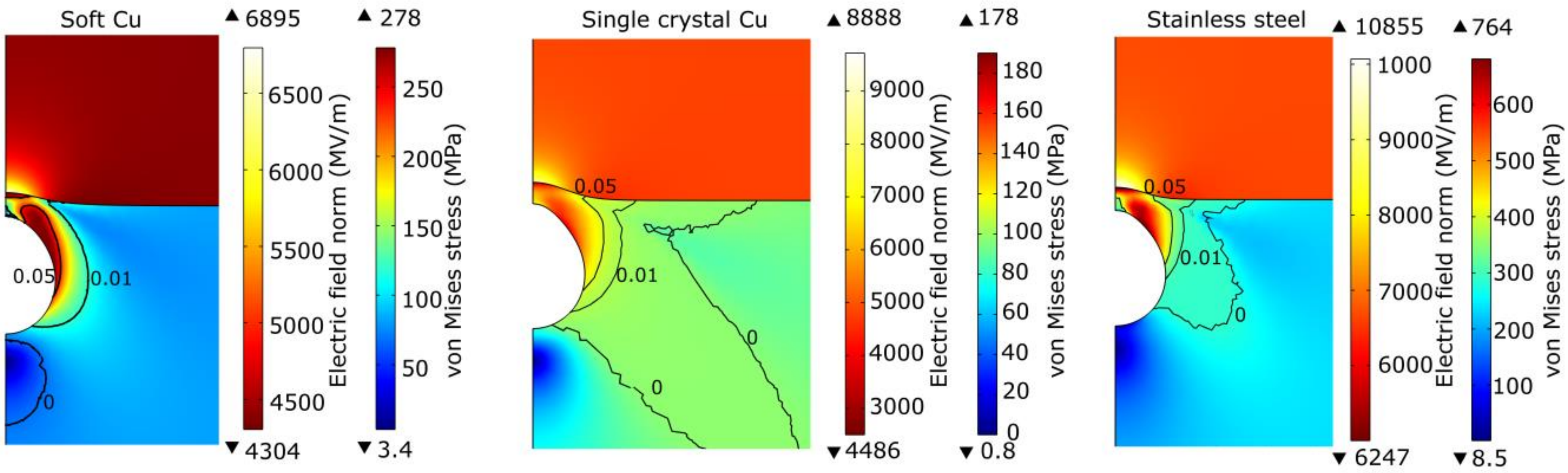
MD vs. FEM in nanoscale

- MD – exaggerated el. fields are needed
- MD simulations are accurate, but time consuming
- FEM is computationally fast, but limited at atomistic scale
- Very similar protrusion shape to MD
- Material deformation starts in same region





Void at max. deformation – different materials

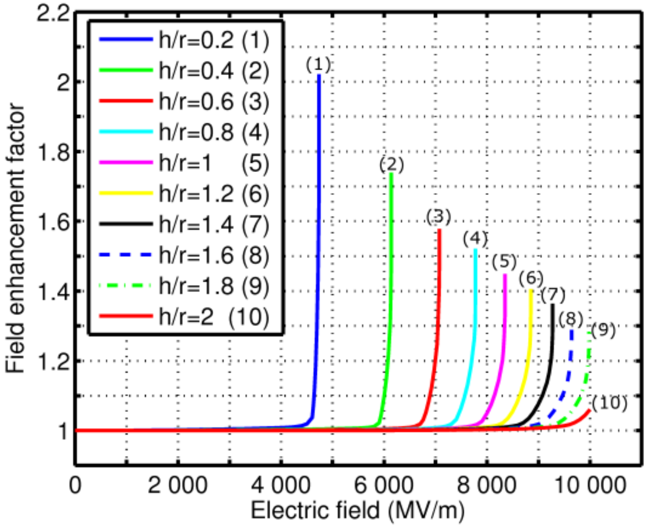


- Similar protrusion shape for all materials
- Higher el. fields are needed to deform stronger materials
- Slightly different maximum stress regions
- Plastic deformation distribution highly dependent from material

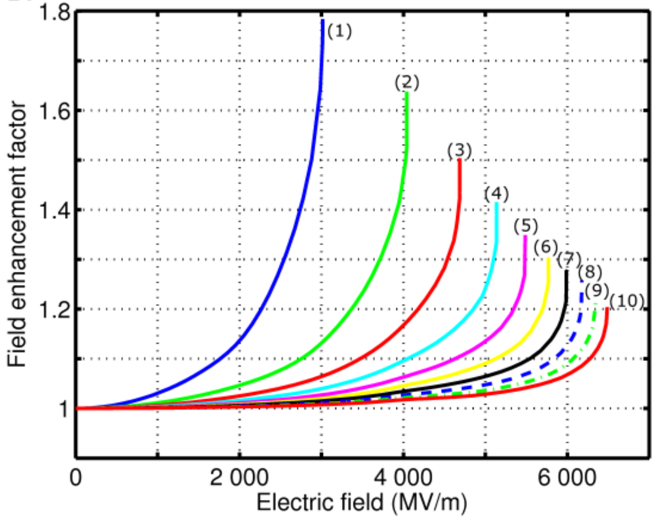
Field enhancement factor

- Field enhancement factor to characterize protrusions shape
- Soft copper
  - Elastic deformation affects field enhancement
  - Field enhancement increasing over whole el. field range
  - Field enhancement is continuous and smooth
- Stainless steel, single crystal Cu
  - Field enhancement almost constant until critical field value
  - Very fast increase of the field enhancement factor
- Maximum field enhancement is 2 times
- Field enhancement corresponds to protrusion growth

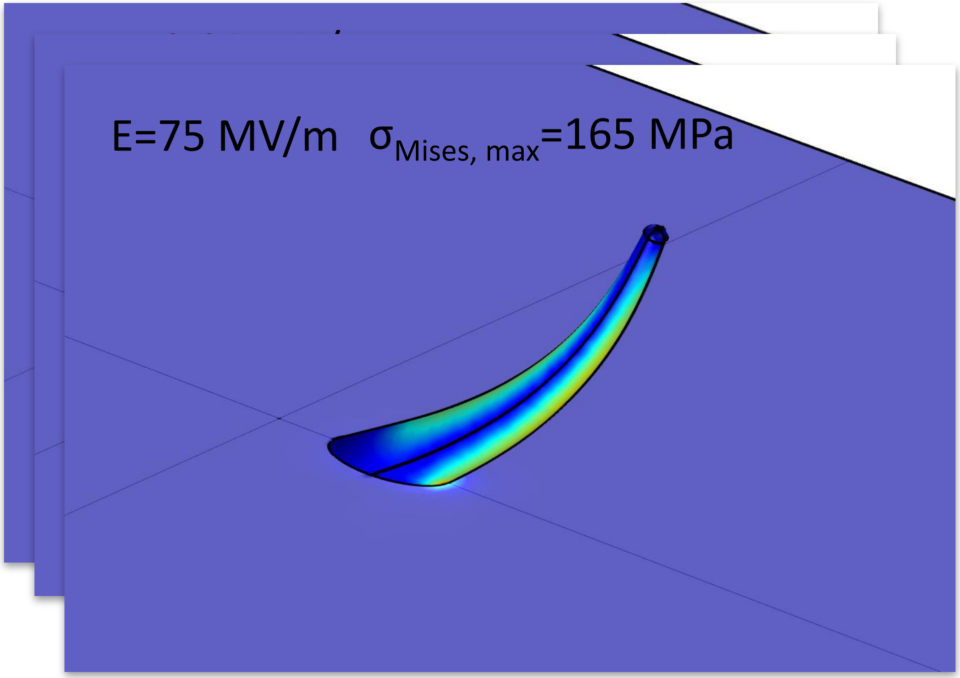
A. Steel



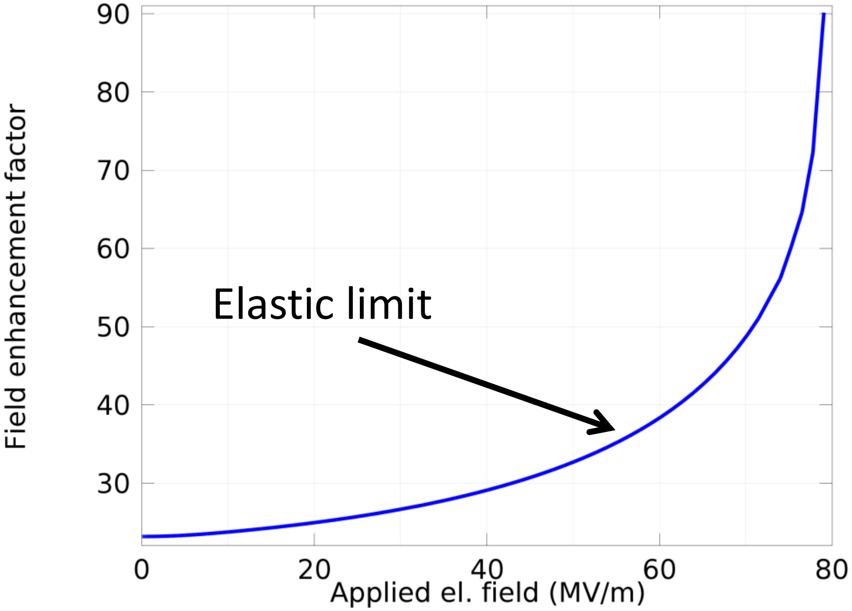
B. Soft Cu



Rising tip in el. field

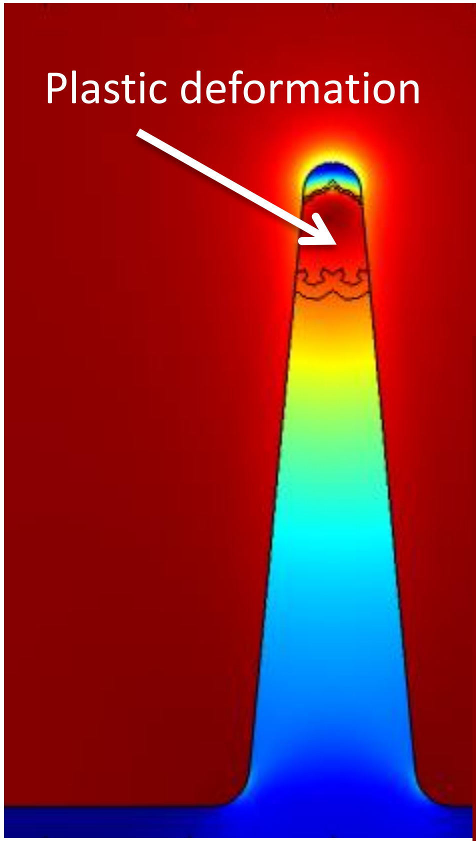


- Field emitting tip, raising from the surface is assumed
- Simulation starts, when the emitter is ~40^{o} angle
- Simulation ends when fast increase of field enhancement factor starts


Elastic limit

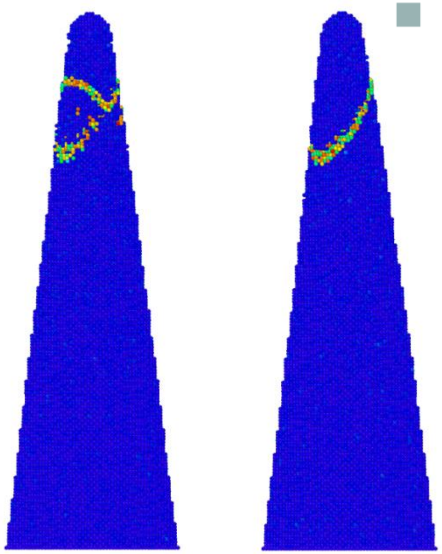
- Dynamic behavior of field enhancement factor
- Elastic deformation up to ~56MV/m
- Corresponding field enhancement factor 35
- Rising tip can cause significant increase of the field enhancement

Single tip deformation

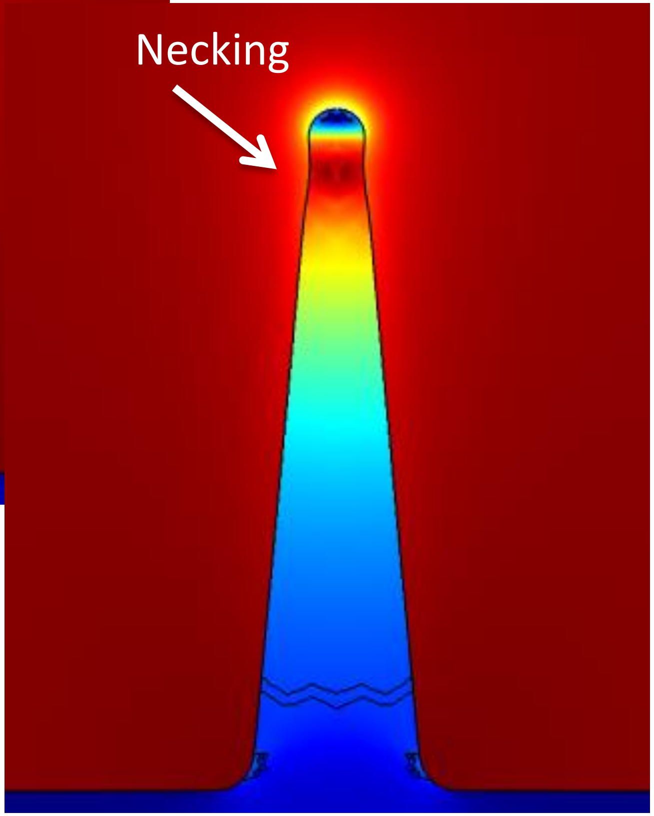


- Plastic deformation in FEM
- Dislocations in MD

- Dislocations are carriers of plastic deformation



FEM overestimates plastically deformed area!

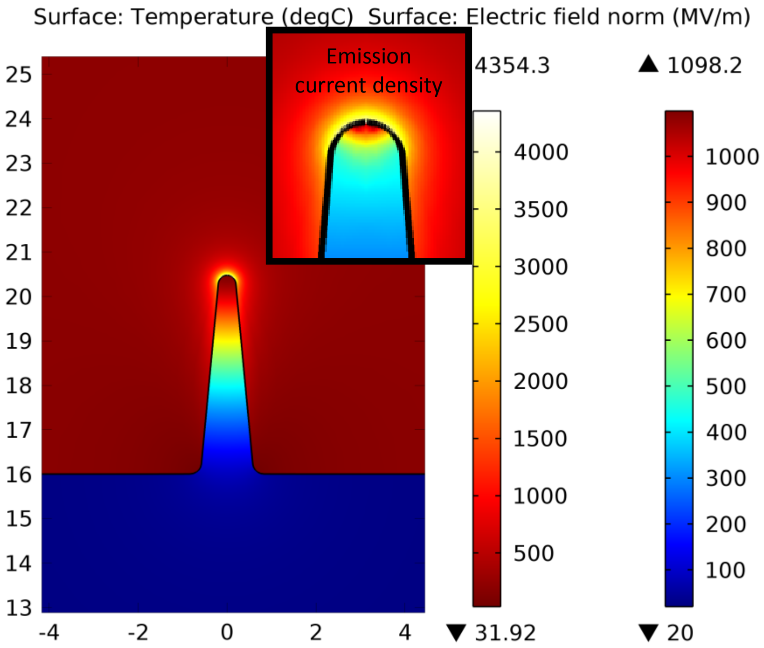


- Nanoscale tip under electric field induced stress
- Simulations with FEM and MD
  - Constant temperature
  - No emission currents
  - Linear ramping of el. field
- MD and FEM predict the same location for plastic deformation
- Piece of material is removed from the tip

Heating and emission currents

Local Fowler-Nordheim eq.
for emission currents –
connection to the experiment

$$\boxed{J = \frac{1.54x10^{6}E^{2}}{\varphi}\exp\left(10.41\ \varphi^{-1/2}\right)\exp\left(-\frac{6.53x10^{3}\varphi^{3/2}}{E}\right)}$$



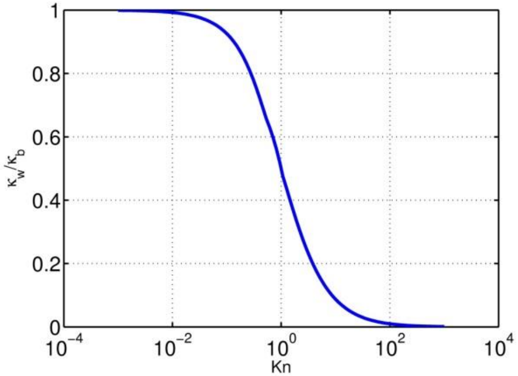
- Fast, exponential temperature rise in the tip
- Emission currents concentrated to the top of the tip
- Melting temperature reached at ~204 MV/m

Field emitters as nanowires

$$\boxed{\sigma_w = F(Kn)\cdot\sigma_b}$$

$$\boxed{\kappa_w = F(Kn)\cdot\kappa_b}$$

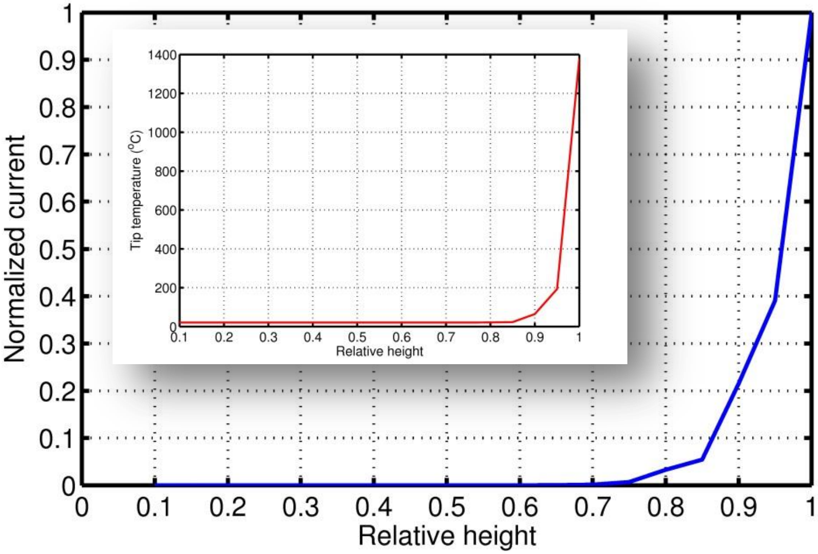
$$\boxed{Kn = \frac{L_{free}}{d}}$$



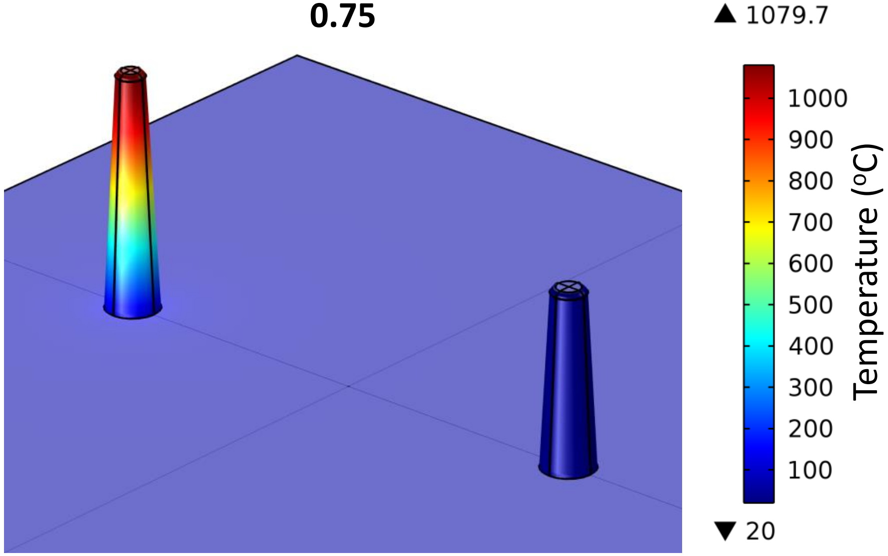
- Size dependence of electric and thermal conductivity
- Conductivity in nanoscale emitters is significantly decreased (more than 10x for sub-nanometer tip)
- Knudsen number to characterizes nanoscale size effects
- Wiedemann-Franz law for thermal conductivity

Selective heating of the tips

- Simulation of two field emitters
  - Emitter 1 – height *H* fixed
  - Emitter 2 – height changed from 0.1*H* to 1*H*
- Ramping of the el. field
- Only the highest tip emits currents
- Significant emission from smaller tip started, when its height was 85%-90% of the largest tip height



Temperature of the tips, relative height 0.75

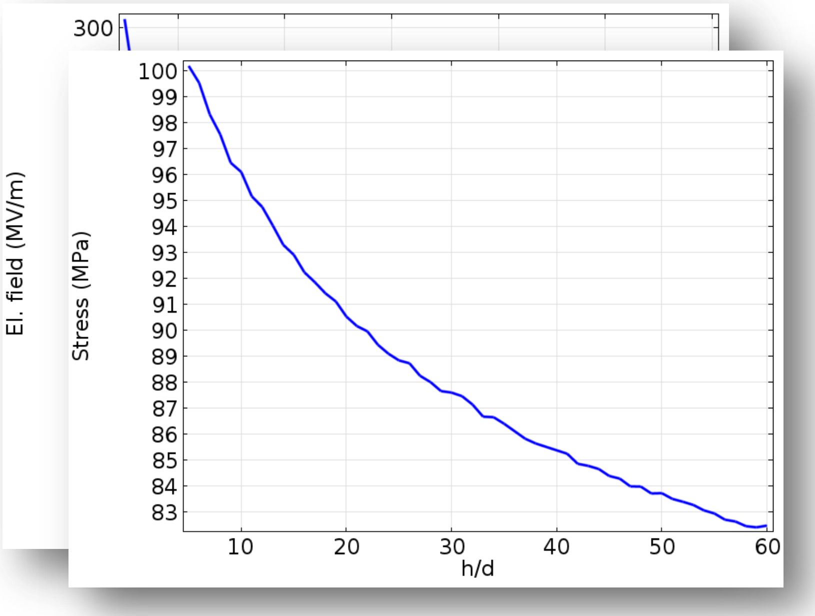


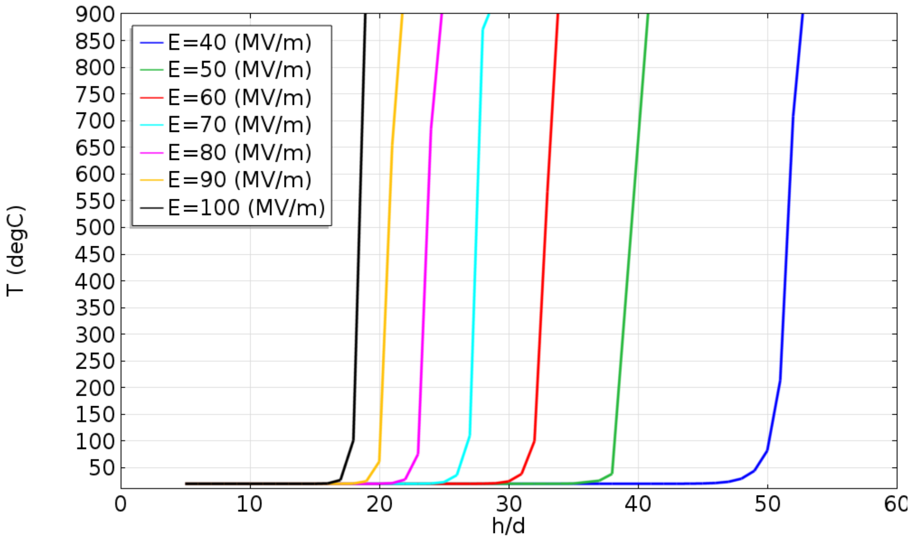
Tip behavior under the el. field:

- only the highest tips start to emit the current, when the field is turned on
- longest tips heat, melt/vaporize, until they shorten to the height of the smaller tips
- finally, all the emitters should have equal height

Single high aspect ratio emitter in electric field

- Simulated emitter aspect ratio 2…60
- Stop condition: 1000 °C reached
- Tip temperature dependence from field
- Mechanical stress due to el. field at simulation stop always over yield strength
- Nonlinear heat and electric conductivity lead to fast decrease of acceptable electric field
- **Limiting case for multiple field emitter simulations**

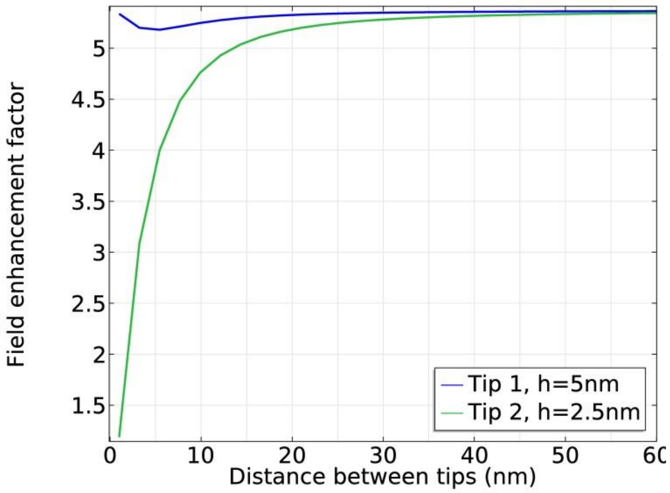


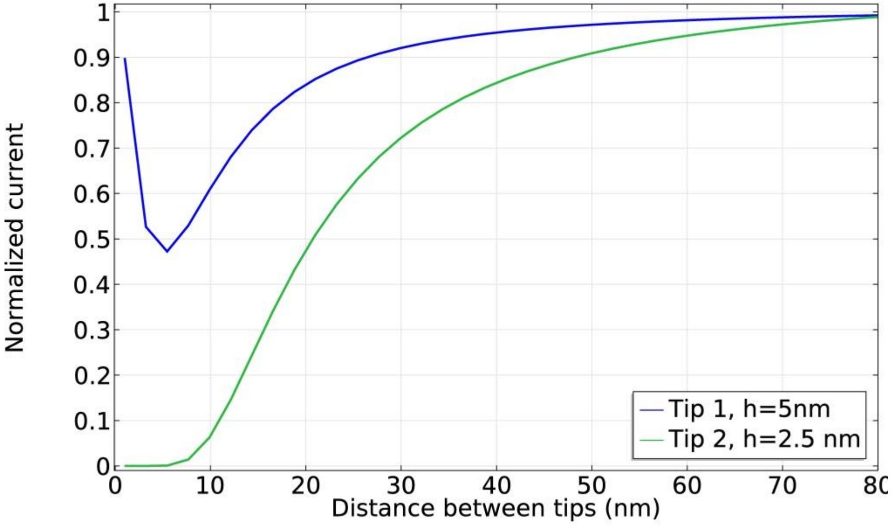


- High temperature dependence from aspect ratio
  - 100 MV/m limited to emitters with aspect ratio below 20
  - Maximum simulated aspect ratio – 60 survives fields up to 40 MV/m
  - **more complex field enhancing surface structures are needed**

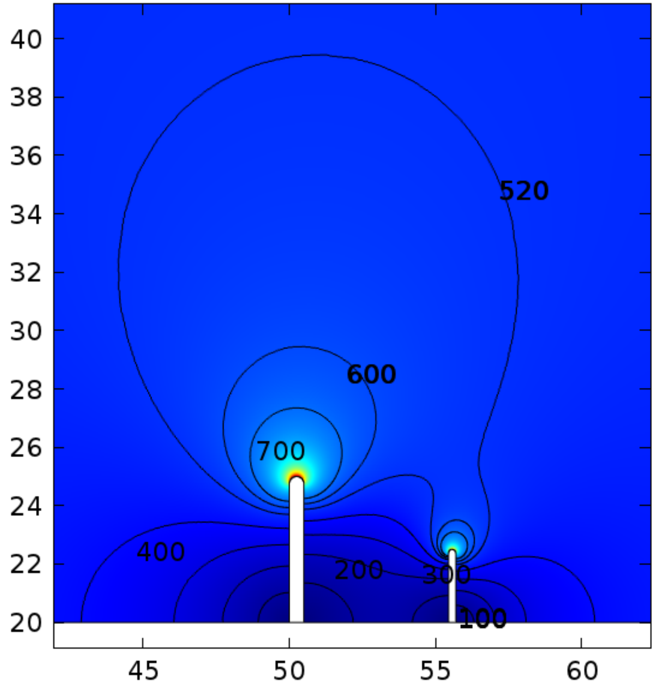
Interaction of emitters at constant field

- **Electric field and emission current density at constant external field (500 MV/m)**
- **Emitters have equal aspect ratio and shape, but different scale (0.5x scaling)**
  - **Equal emission current density expected**
- Close emitters act as single one
- The field enhancement factor of smaller tip is affected up to the Tip separating distances 30-40 nm – 6-8 times of the height of the largest tip
- The emission current densities from both tips are affected up to distances between the tips 60-70 nm – more than 10 times the height of the larger tip
- The emission current from the smaller tip is reduced 2 times if, the distance between the tips is 20 nm (4 times the height of larger tip)

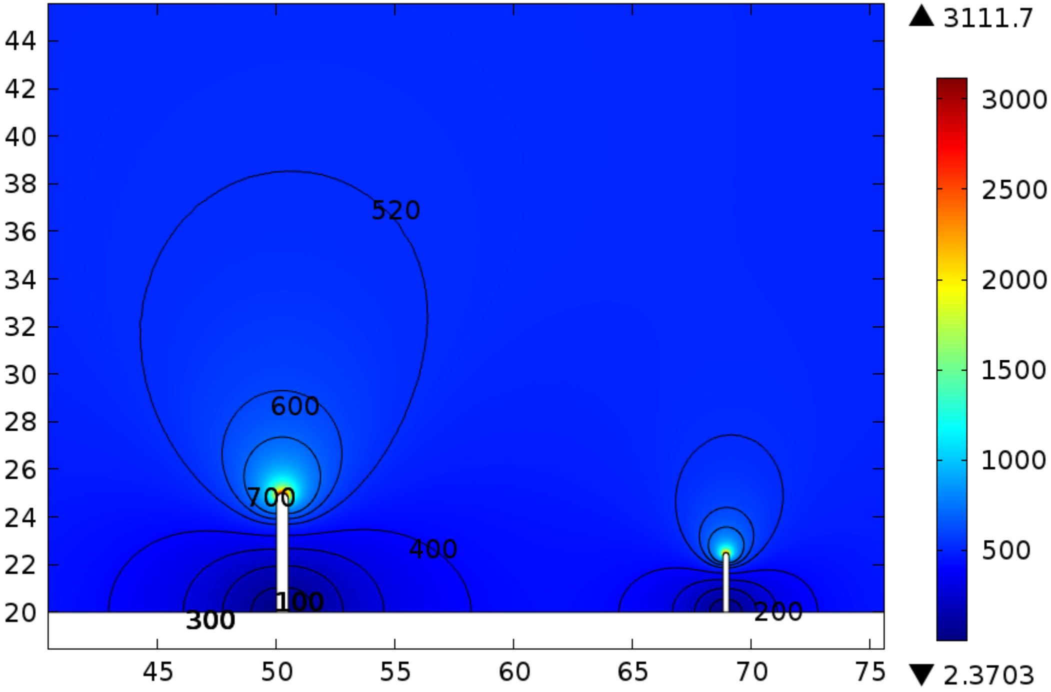




Electric field distribution due to interacting emitters



- Small emitter „captures“ part of the field from large emitter
- Smaller emitter is located in the low field region, created by tall emitter

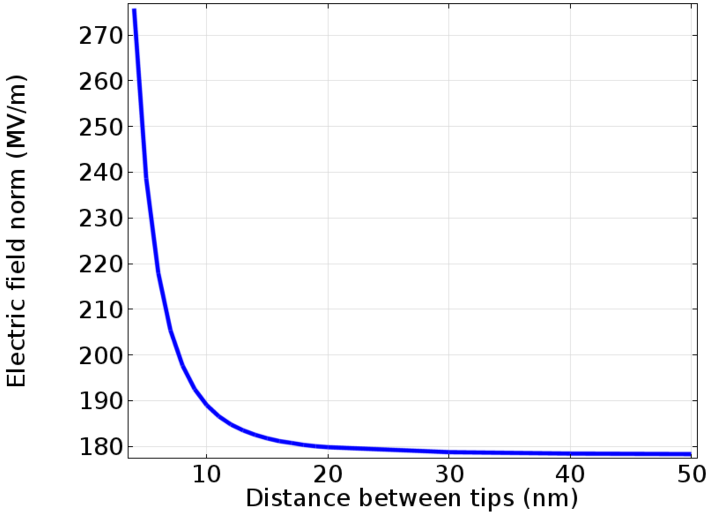


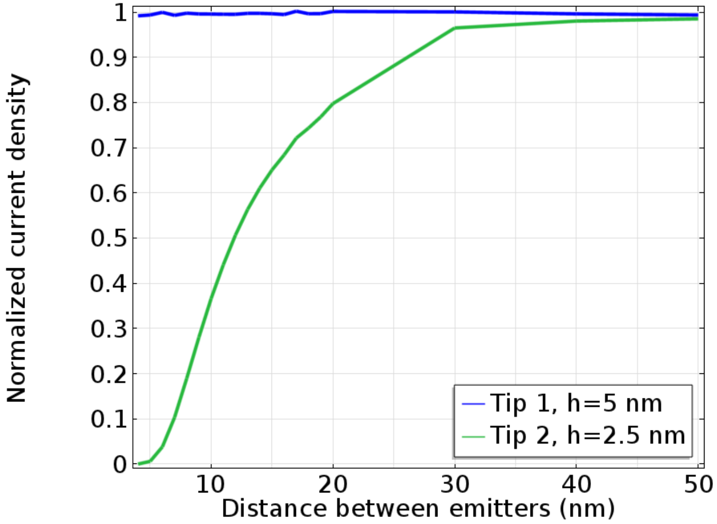
- Emission current sensityvity to the applied field
- **Local interactions on surface can have signifficant effect to the breakdowns**

Interaction of the emitters – the breakdown limit

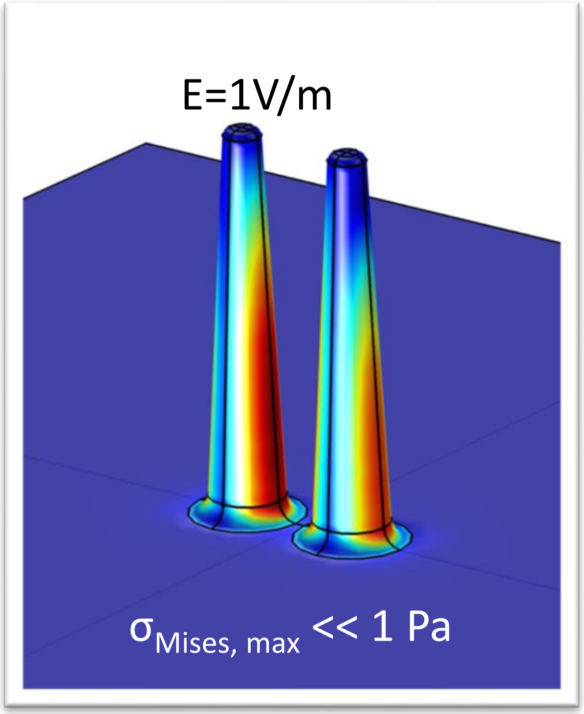
- Electric field and emission current density at the breakdown condition (1000 °C reached in any emitter)
- Simulated emitters have equal aspect ratio, but different scaling (0.5x)

- Significant apex el. field and emission current density reduction at smaller tips
  - Shielding effect of larger emitters
  - 50% reduction of emission current density in ~13 nm from taller tip (2.6x height)
  - Shielding effects disappear at 30 nm emitter separating distance
- **Can we use artificial „emitters“ to control the breakdowns?**





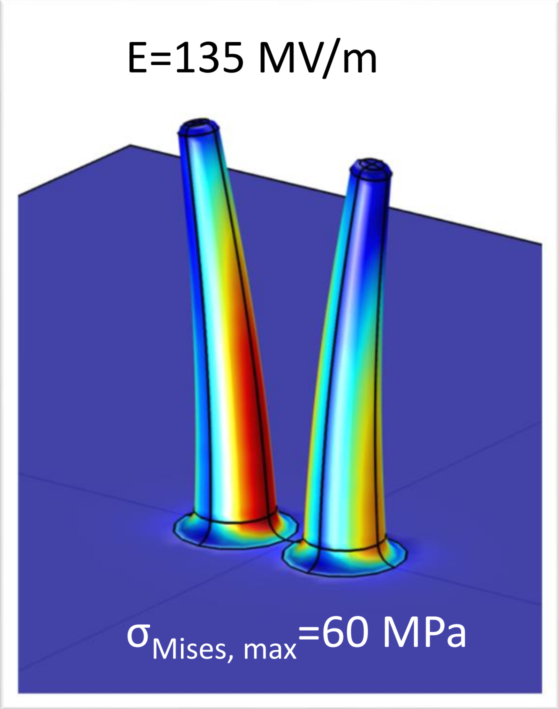
Mechanical interactions of emitters



- Two closely located emitters
- Emitter aspect ratio ~10
- Distance between the emitters – 0.3*H* (*H* – height of the emitter)
- Linear ramping of el. field

Elastic regime:

- Reversible deformation of the emitters

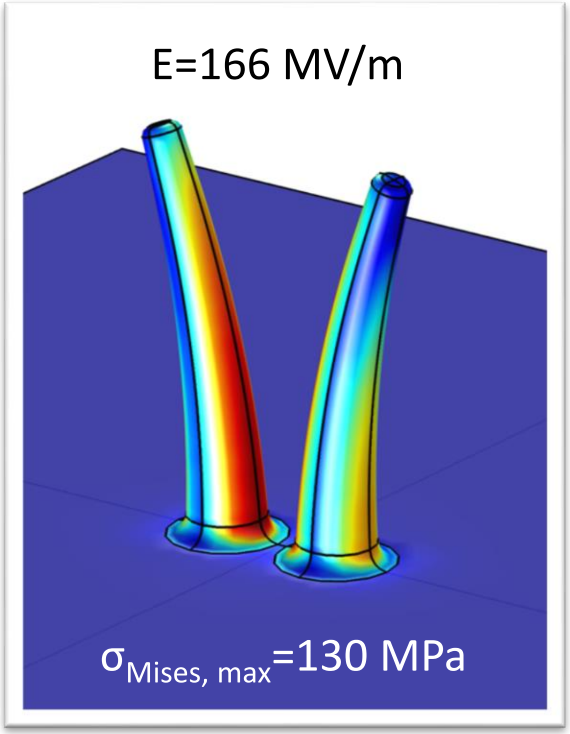


Nearby emitters interact

The emitters repel due to the surface charge

Plastic regime:

- Highest stress is at inner side of the tip
- Limiting effect to the density of emitters?



Conclusions

- FEM is a viable tool to simulate material defects
  - MD is still needed to determine physics behind the effects
- Local interactions between the emitters can have significant influence to emission currents
  - Possibilities for controlling the breakdowns
- Near field emitters interact due to surface charge
- Significant field enhancement by rising emitter
- Only the highest tips emit currents
  - Emitting tips are with equal height

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