Multiphysics simulations of surface under electric field

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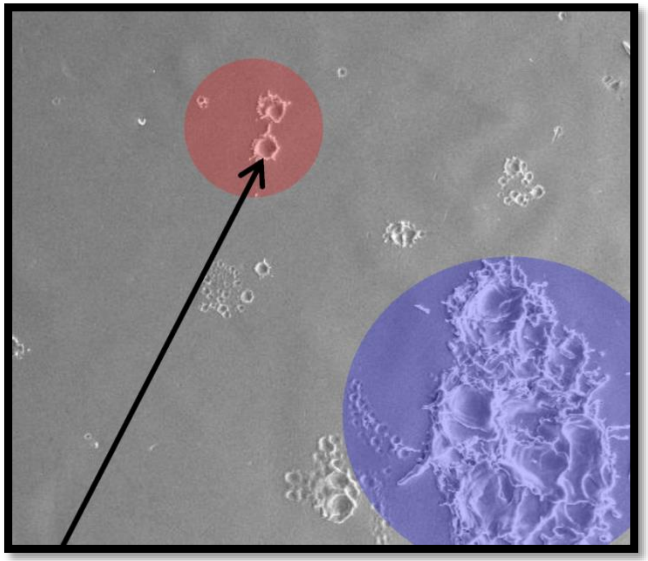
Electrical breakdowns

Electrical breakdowns at CLIC accelerating structure materials

Accelerating gradients 100-150 MV/m



M. Aicheler, MeVArc 2011

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

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

Voids in the material as possible factors affecting surface defects

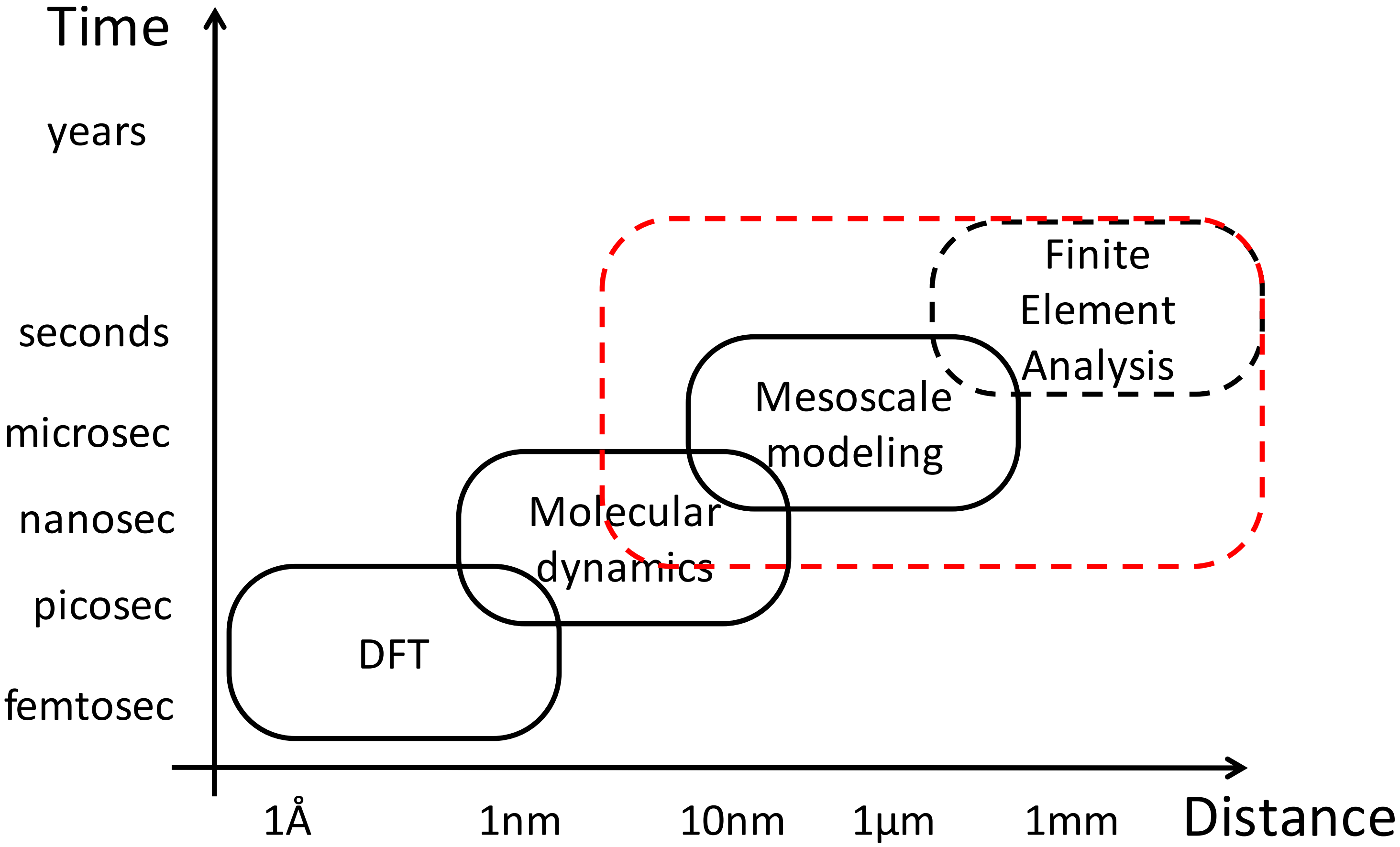
Void hypothesis

- A void as a possible mechanism for generating a field emitter
  - Void in material is a stress concentrator
    - Voids are spherical due to surface energy minimization
    - In hypothesis we consider a single void in metal
  - We aim to understand a protrusion growth mechanism in the case of spherical void in DC electric-field

- Several mechanisms acting at once to produce a tip?
  - May be, but for now we focus on one

- Field emitters as initiators of a breakdown
  - Thermal-electrical behavior of field emitters
  - Mechanical behavior of field emitters

Computer simulations in Chemistry and Physics



Time

years

seconds

microsec

nanosec

picosec

femtosec

DFT

Molecular dynamics

Mesoscale modeling

Finite Element Analysis

1Å

1nm

10nm

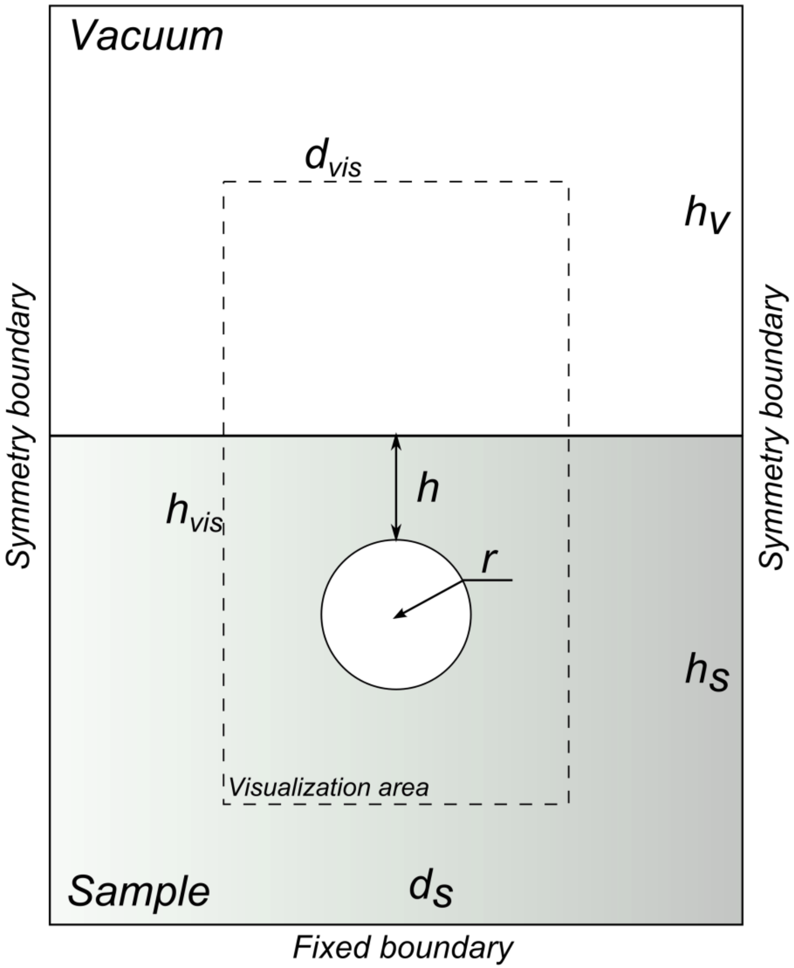
1µm

1mm

Distance

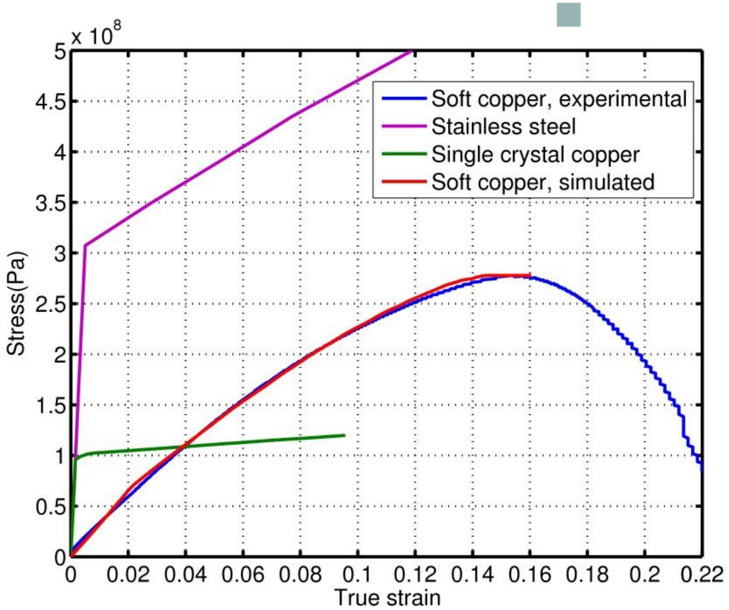
Simulated system

- Fully coupled electric field – elastoplastic interaction
  - Electric field deforms sample
  - Deformed sample causes local field enhancement
- Dc El. field ramped from 0 … 10 000 MV/m
- Comsol Multiphysics 4.3b
  - Nonlinear Structural Materials Module
  - AC/DC module
- 3D-simulations, 2D-snapshots
- Simulated materials:
  - Soft copper
  - Single crystal copper
  - Stainless steel



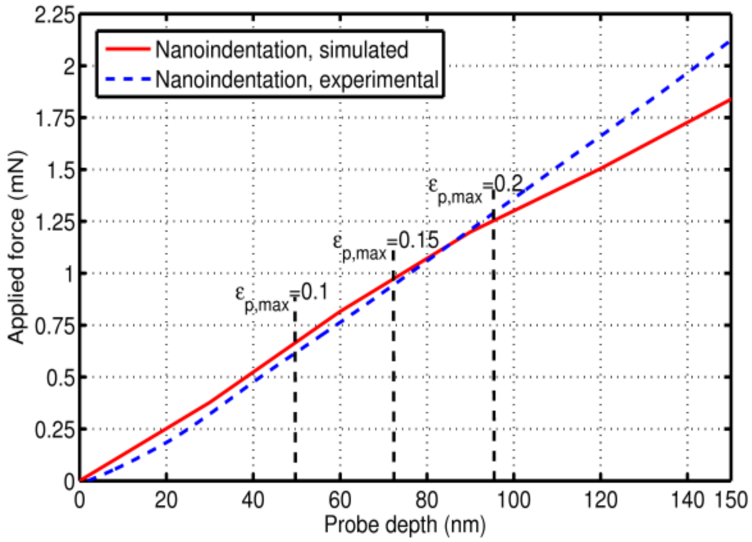
Material model

- 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**



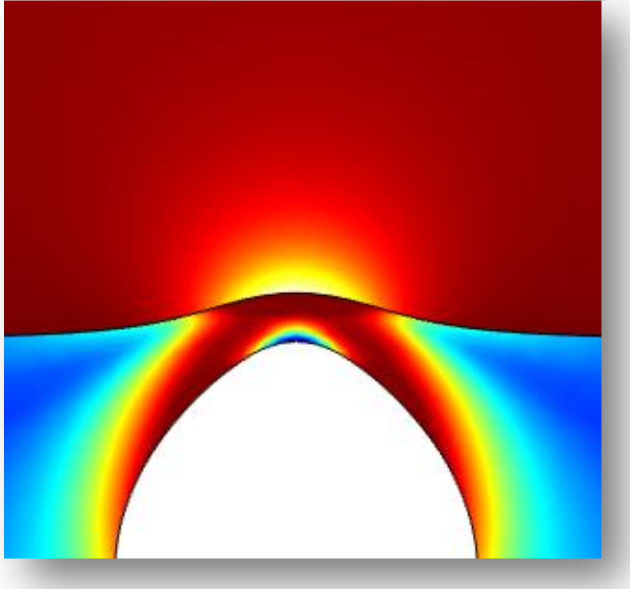
	Structural Steel	Soft Copper (CERN)	Single crystal copper [1]	Often used copper parameters
Young's modulus	200 GPa	3.05 GPa	57 GPa	110 GPa
Initial yield stress	290 MPa	68 MPa	98 MPa	70 MPa

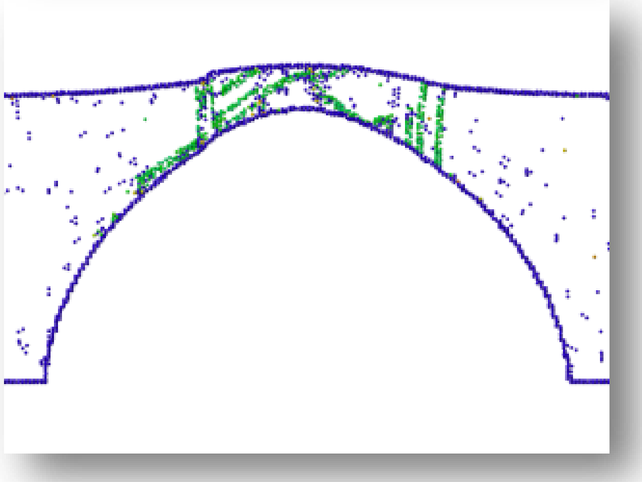
[1] Y. Liu, B. Wang, M. Yoshino, S. Roy, H. Lu, R. Komanduri, J. Mech. Phys. Solids, 53 (2005) 2718



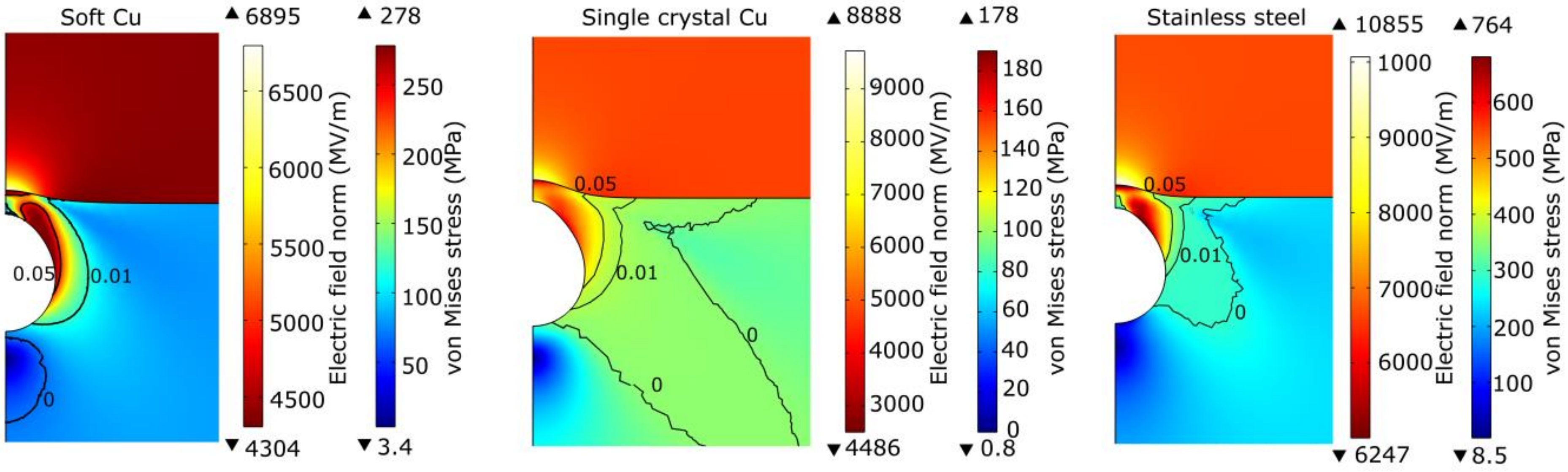
MD vs FEM

- 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
- Material deformation starts in same region





Void at max. deformation – different materials

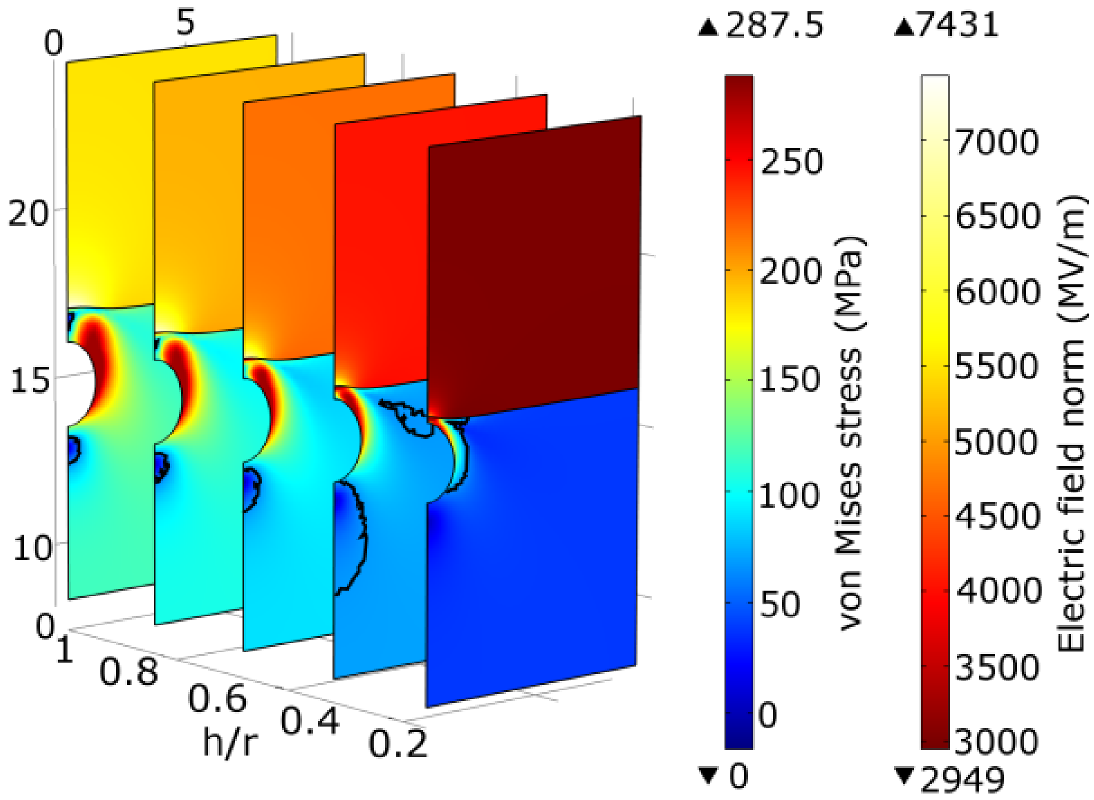


- Similar protrusion shape for all materials
- Higher el. fields are needed to deform stronger materials
- Slightly different maximum stress regions
- Plastic deformation distribution highly dependent from material

Protrusion formation at different depths

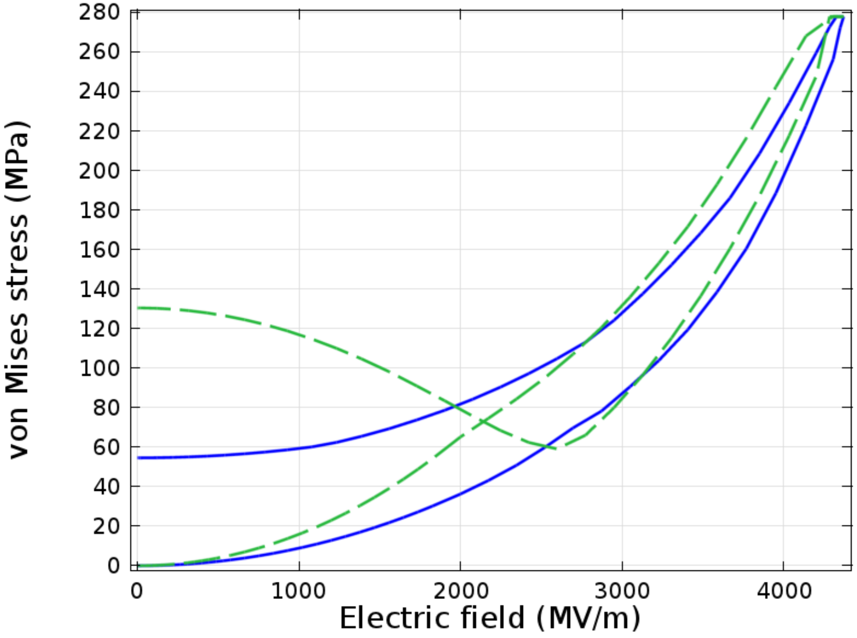
- Close to surface void needs smallest el. field for deformation
- Max. stress for near surface voids is concentrate between void and sample surface
- Max. stress distribution moves to the sides of void by increasing depth
- Deeper voids cause whole material to deform plastically

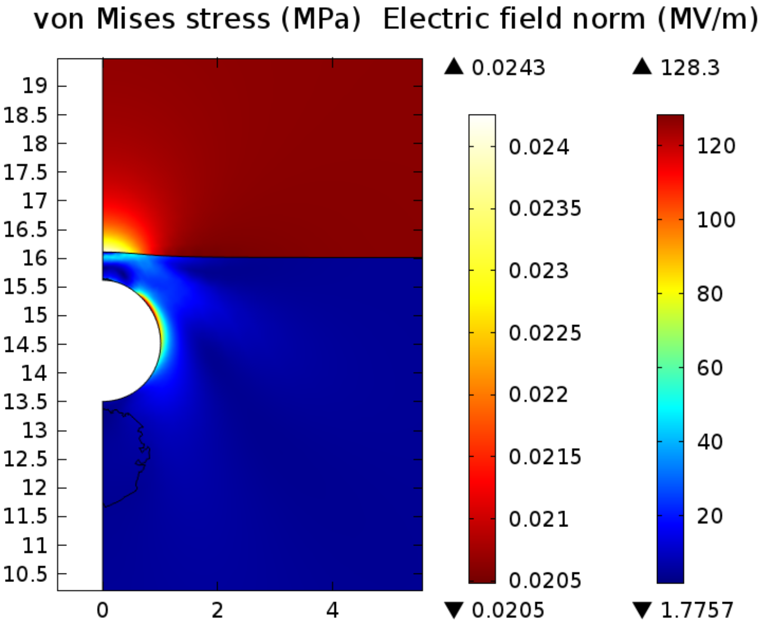
Soft Cu



Cycling the voltage

- Cycling of the material under electric field
- Soft copper, spherical void, with h/r=0.5
- Electric field ramped up to 2500 MV/m -> 0 MV/m
- Field is ramped until ultimate tensile strength is reached



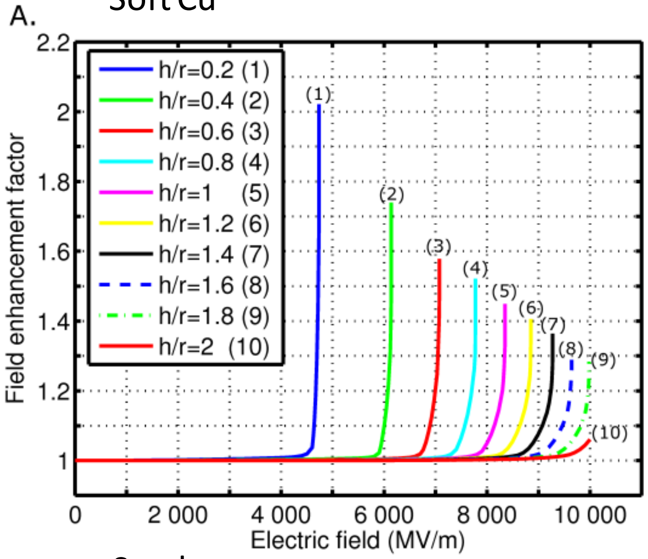


- Protrusion almost completely retracted after unloading
- Very high residual stress after unloading
  - Initial yield stress ~70 MPa
- Stress at void surface considerably higher than at material surface
- Complex evolution of stress distribution during unloading

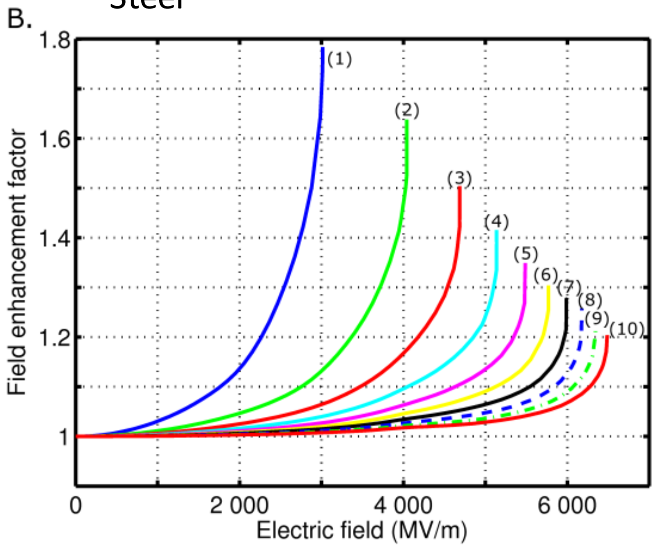
Field enhancement factor

- 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

Soft Cu

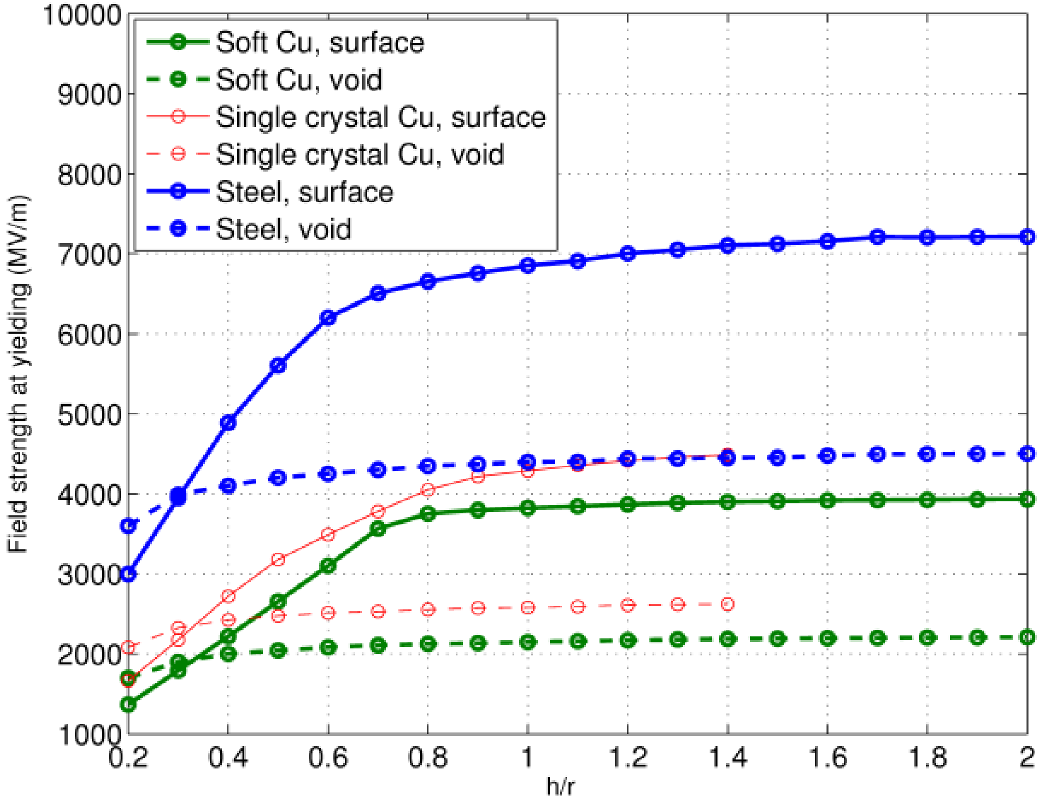


Steel



Yield point

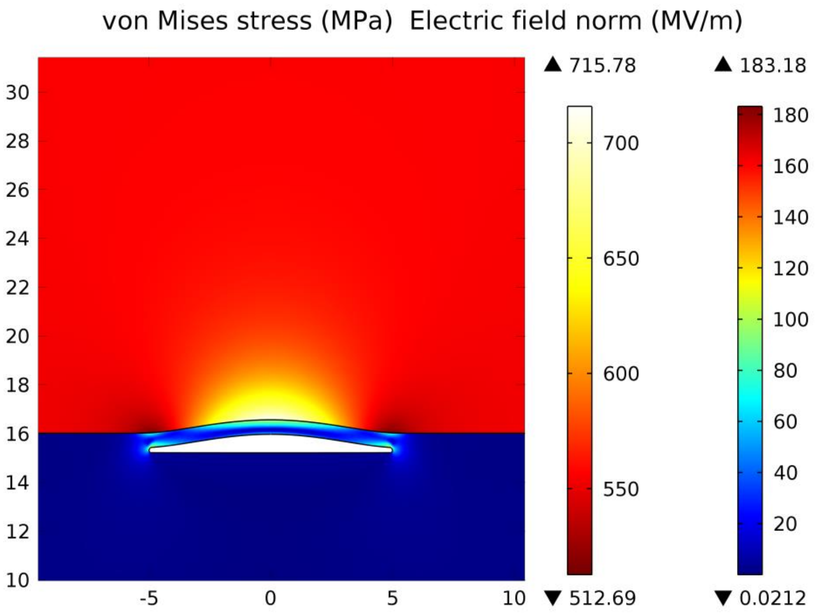
- Nonlinear dependence from the void depth
- For **h/r<0.3**, yielding starts at void tip
- For **h/r=0.3**, yielding equal at tip and sides
- For **h/r>0.3**, stress is carried to the sides of the void
- Three deformation mechanisms
  - Deformation at metal surface
  - Deformation at void surface
  - Deformation due to decreased surface area
- Too deep void starts to decrease the effective surface area of the sample



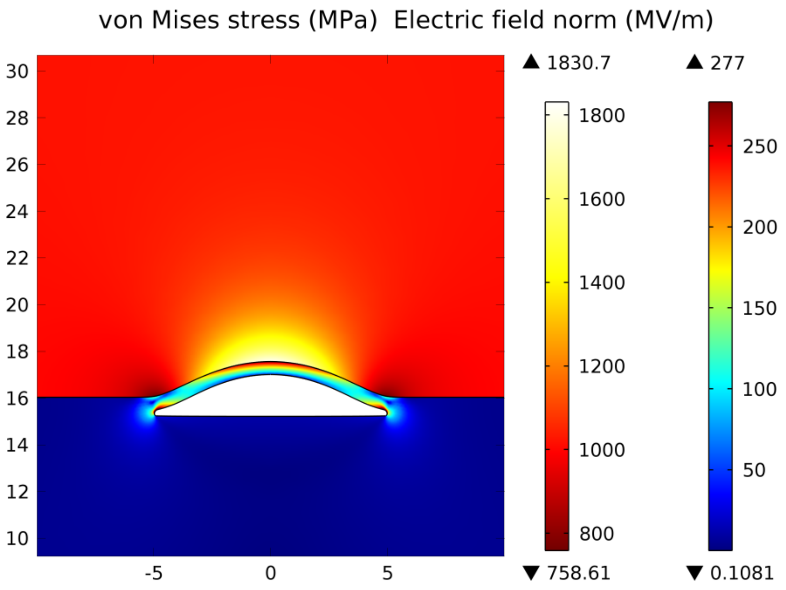
- Steel
- Single crystal copper
- Soft copper

Deformation at realistic electric field strength

- Void formation starts at fields > 400 MV/m
- Material is plastic only in the vicinity of the defect
- Thin slit may be formed by combination of voids or by a layer of fragile impurities



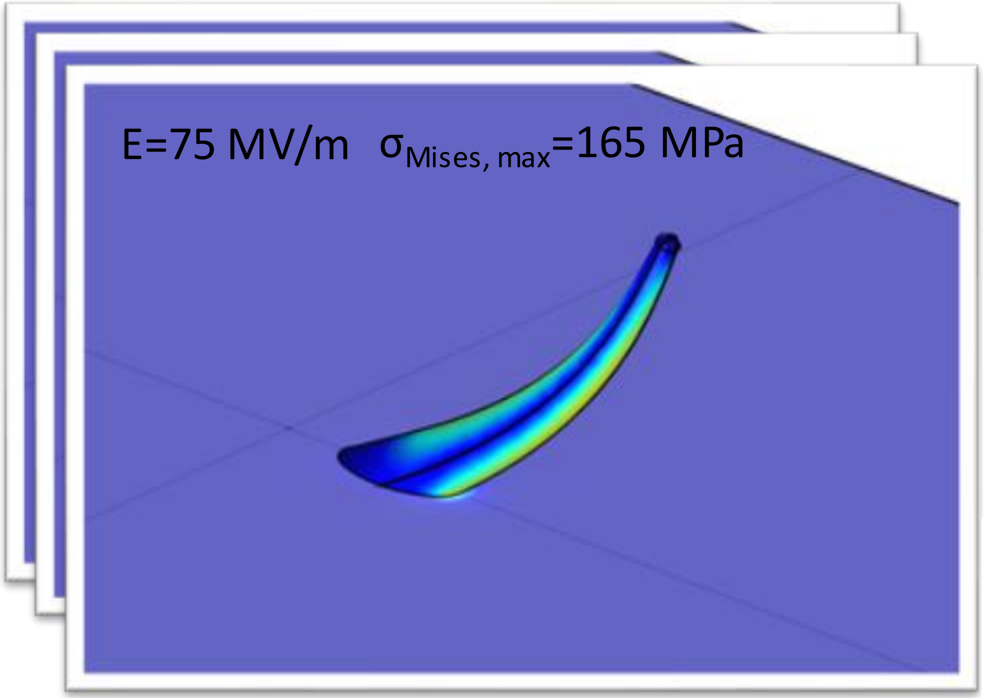
von Mises stress (MPa) Electric field norm (MV/m)



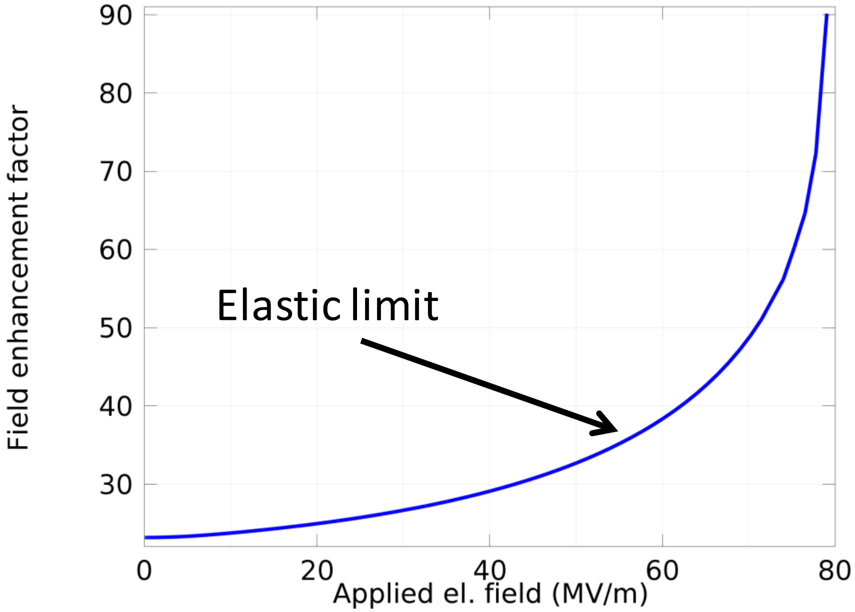
von Mises stress (MPa) Electric field norm (MV/m)

- Field enhancement factor ~2.4
- Thin material layer over the void acts like a lever, decreasing the pressure needed for protrusion formation

Rising tip in el. field



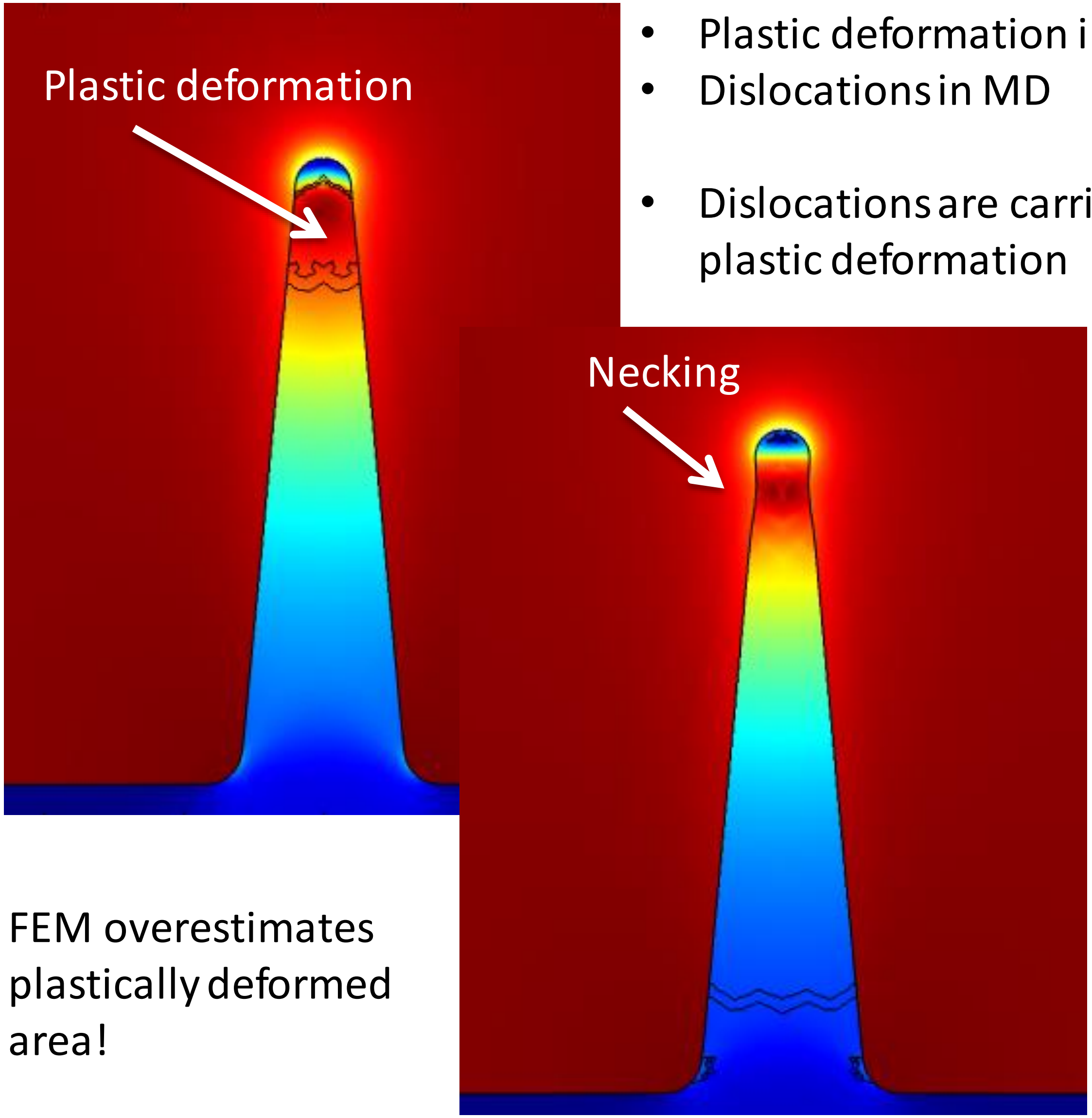
- Field emitting tip, raising from the surface is assumed
- Simulation starts, when the emitter is ~40^{o} angle
- Simulation ends when fast increase of field enhancement factor starts



Elastic limit

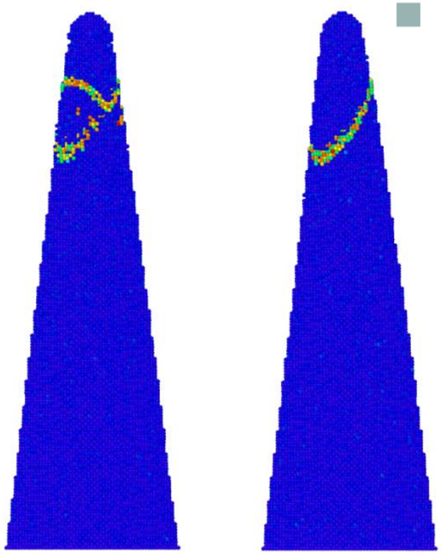
- Dynamic behavior of field enhancement factor
- Elastic deformation up to ~56MV/m
- Corresponding field enhancement factor 35
- Raising tip can cause significant increase of the field enhancement

Single tip deformation



- Plastic deformation in FEM
- Dislocations in MD

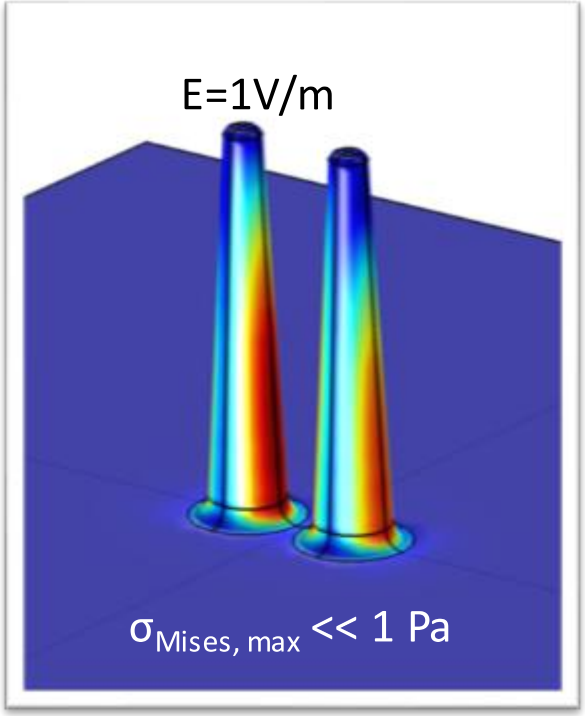
- Dislocations are carriers of plastic deformation



- 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

FEM overestimates plastically deformed area!

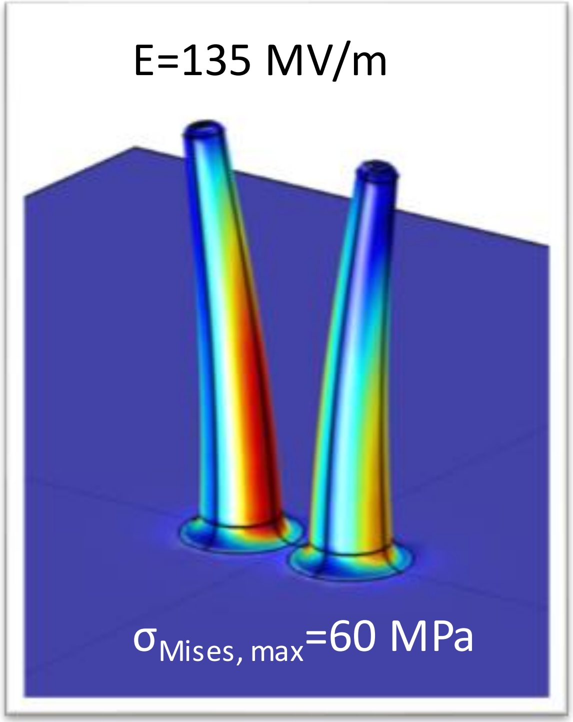
Interacting emitters



- 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

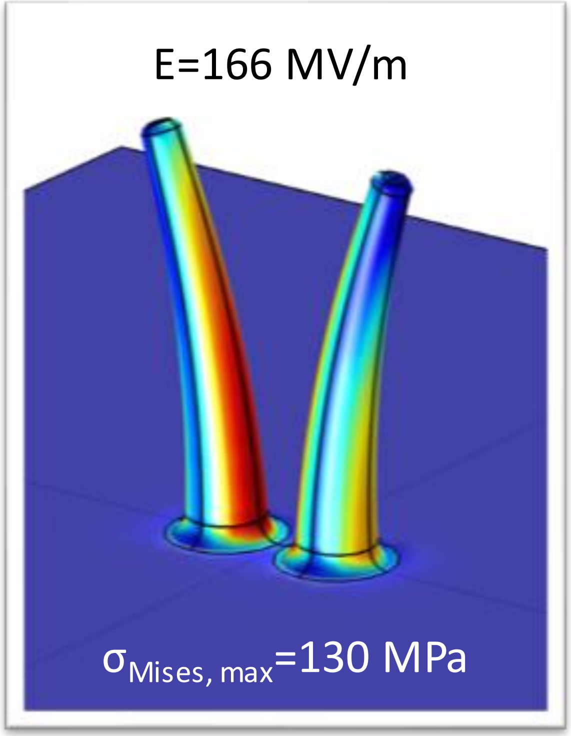


Nearby emitters interact

The emitters repel due to the surface charge

Plastic regime:

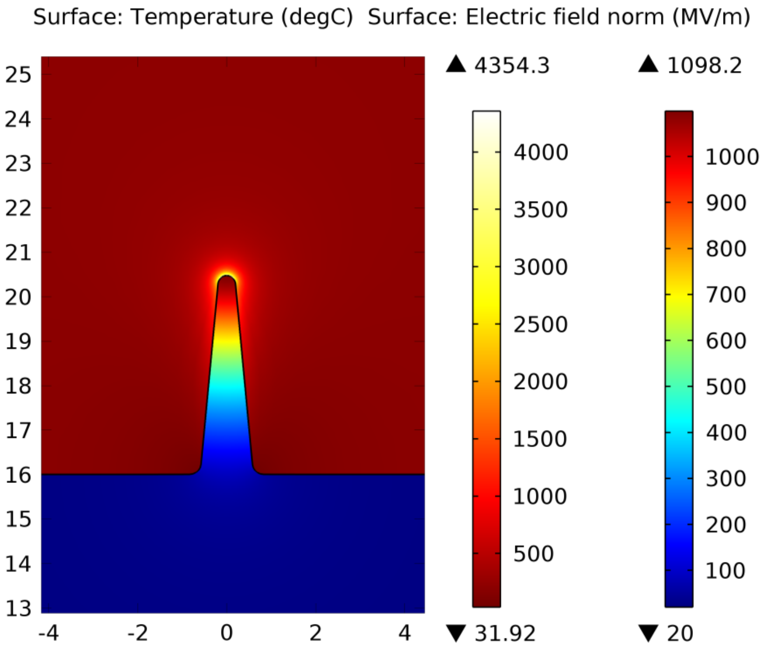
- Highest stress is at inner side of the tip
- Limiting effect to the density of emitters?

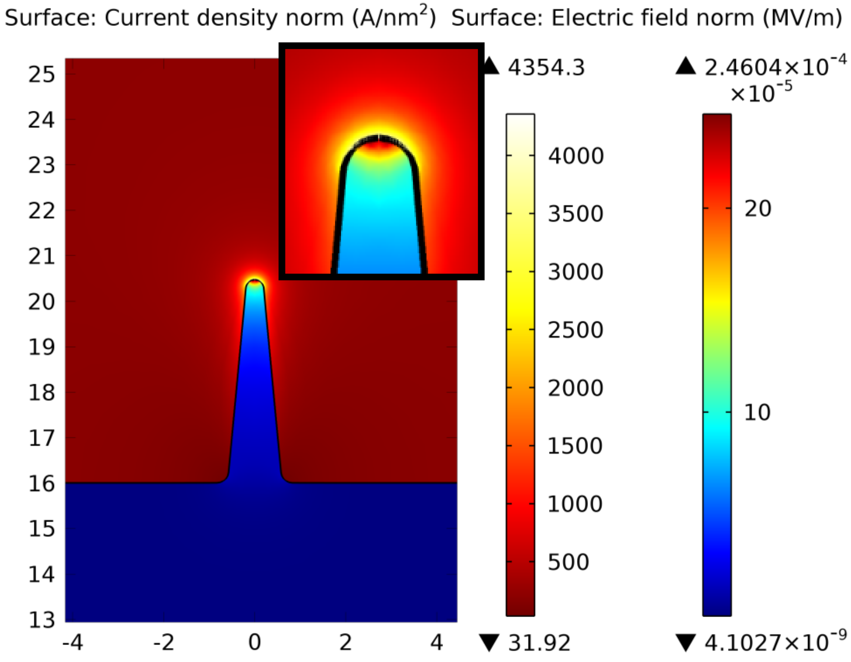


Heating and emission currents

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

$$I = A_e \frac{1.54x10^6(\beta\cdot E)^2}{\phi}\exp\left(10.41\,\phi^{-\frac{1}{2}}\right)\exp\left(-\frac{6.53x10^3\,\phi^{\frac{3}{2}}}{\beta\cdot E}\right) = \xi\,E^2\exp\left(-\frac{\gamma}{E}\right)$$

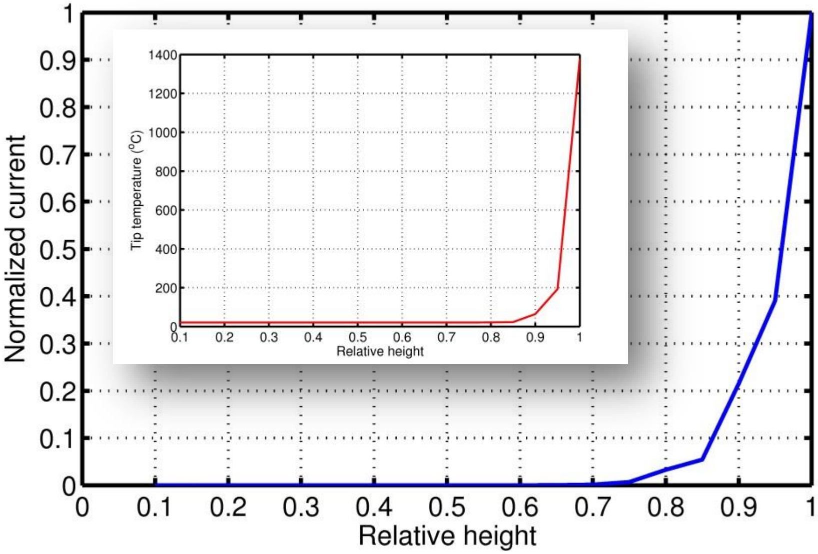




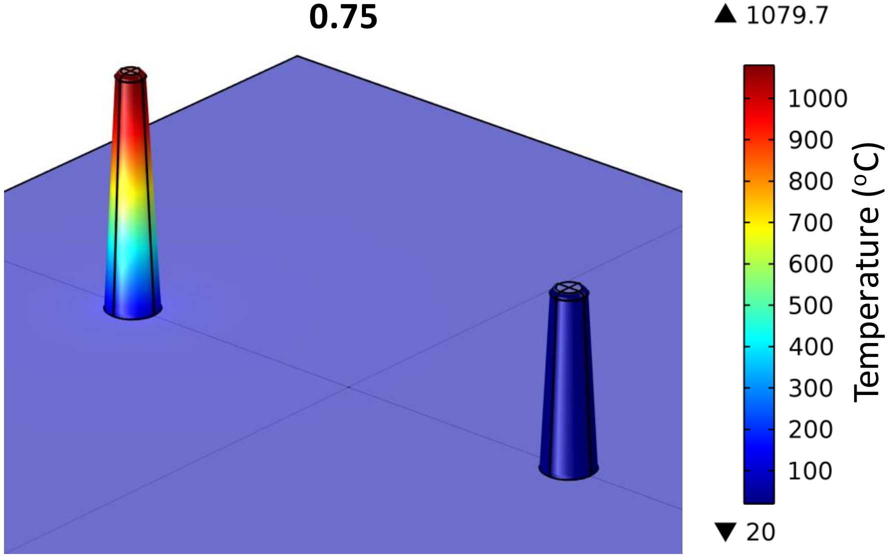
- Fast, exponential temperature rise in the tip
- Emission currents concentrated to the top of the tip
- Melting temperature reached at ~204 MV/m
- Emission current localized to the „tip of the tip“

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:

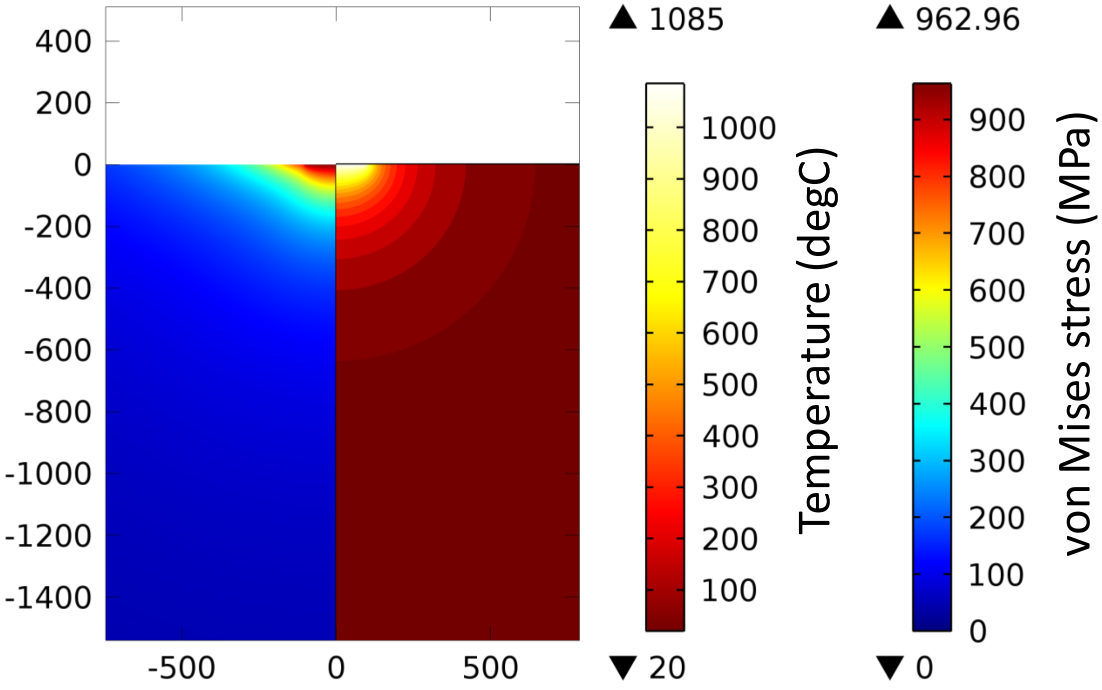
- only the highest tips start to emit the current, when the field is turned on
- longest tips heat, melt/vaporize, until they shorten to the height of the smaller tips
- finally, all the emitters should have equal height

Material heating during the breakdown

- Surface temp. of breakdown spot – melting temp. of copper
- Radius of breakdown spot – 100µm
- Thermal expansion and corresponding stress are calculated

- Fast heating of the material
- Thermal expansion generates large stresses
  - Stress significantly larger than yield strength or ultimate tensile strength of copper
  - Formation of large plastically deformed area around the breakdown spot

Temperature 1 ns after the start of the discharge



Can thermal expansion and resulting plastic deformation produce the conditions required for repeated breakdowns?

Conclusions

- FEM is a viable tool to simulate material defects
  - MD is still needed to determine physics behind the effects
- Protrusion shape is similar for all simulated materials
- Significant material deformation starts after exceeding yield strength
- Field enhancement corresponds to protrusion growth
- Three protrusion generation mechanisms
  - Deformation mechanisms change at h/r~0.3 and h/r~ 1
- Near field emitters interact due to charging
- Significant field enhancement by rising emitter
- Only the highest tips emit currents
  - Emitting tips are with equal height

Thank You for Your attention!

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