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# Thermo-electrical simulations of field emitters - the influence of Nottingham effect

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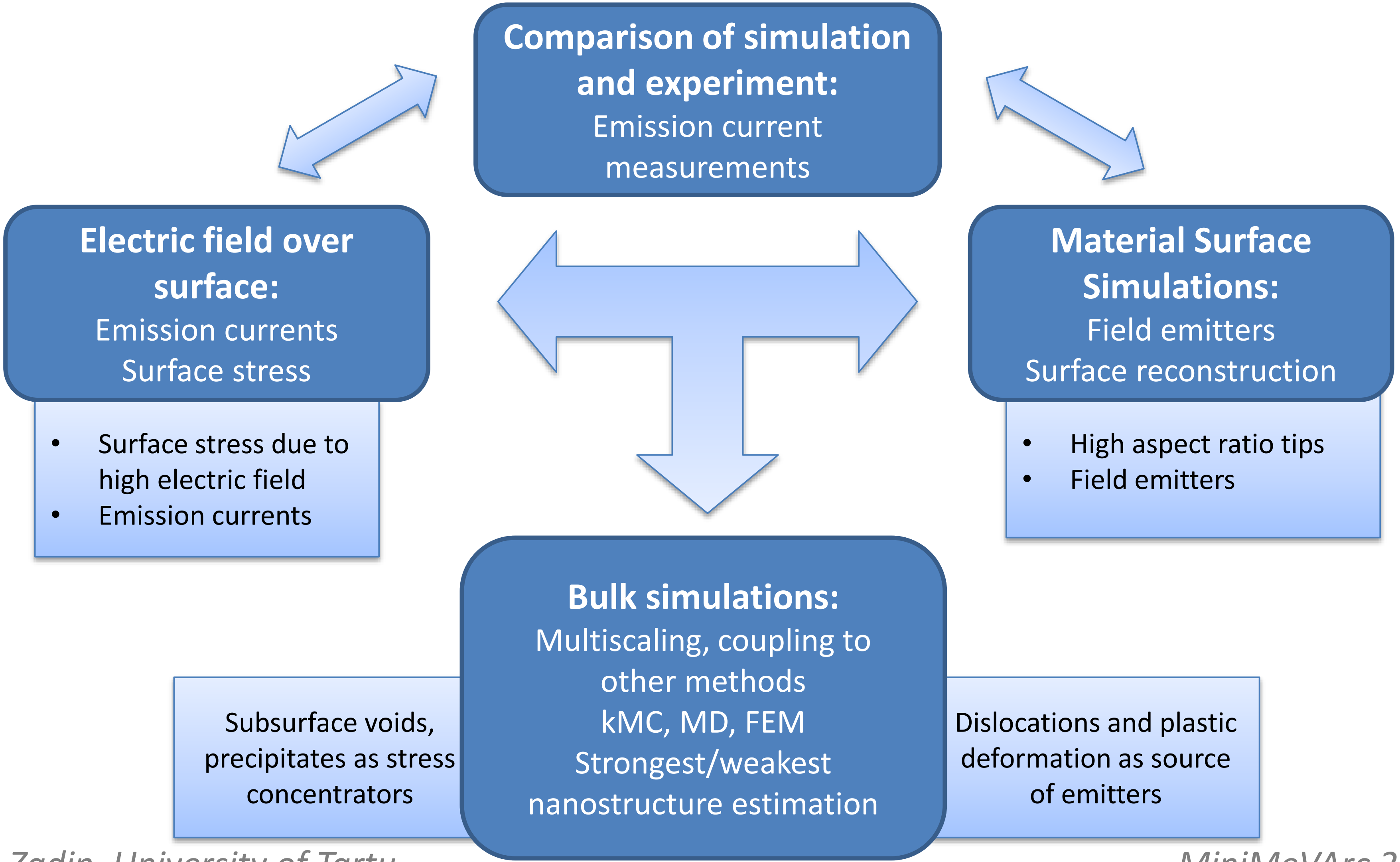
# FEM simulations of field emitters



**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

# Main factors affecting the emission currents

- Possible reasons behind high beta values

**Behavior of single emitter**

- System is always static
- Assumptions for FN theory always fulfilled

**Behavior of system of emitters**

- System is always static
- Multiple emitters, possibly affecting each other
- Assumptions for FN theory always fulfilled

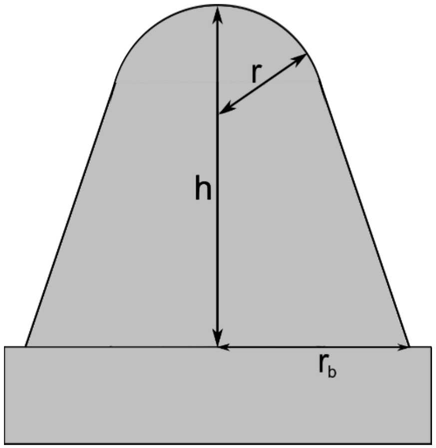
**Integral behavior and surface dynamics**

- Static system in all local configurations
- Changes in system in time or during field ramping
- Possible mechanisms leading to apparent high beta

Nottingham effect – significant contribution to emitter heating and to the dynamic behavior

# 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**
- Nonlinear Structural Materials Module
  - AC/DC module
- HELMOD (Combined Electrodynamics, Molecular dynamics)
- LAMMPS
- Kimocs (by Ville Jansson)
- Simulated materials: Copper

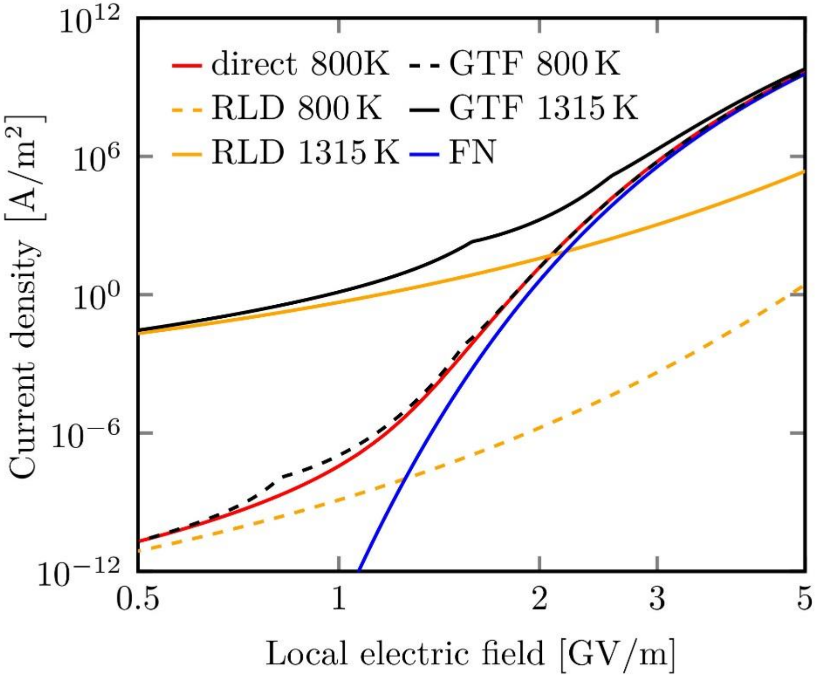
$$r = (2, 4, 8, 16) nm$$

$$h/r = (4, 8, 12, 16, 20)$$

$$r_b/r = (0.2, 0.5, 1.0, 4.0)$$

# 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

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

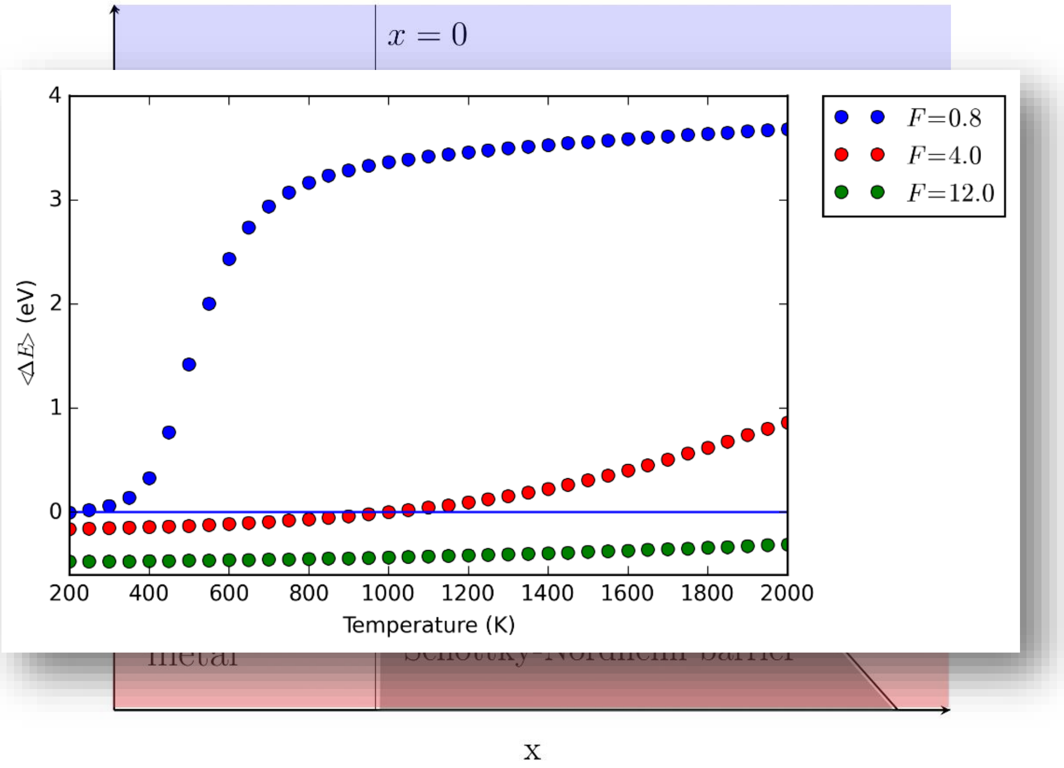
# The Nottingham effect

- Electrons emitted may either cool or heat (depends on the energy) the metal surface.
- The Nottingham effect is characterized by the average energy difference from Fermi energy of the emitted electrons:

$$\langle \Delta E \rangle = \frac{q \int (E-\mu) D(E,F) N(E,T) dE}{j(F,T)}$$

$$\langle \Delta E \rangle > 0 \rightarrow \text{cooling}$$

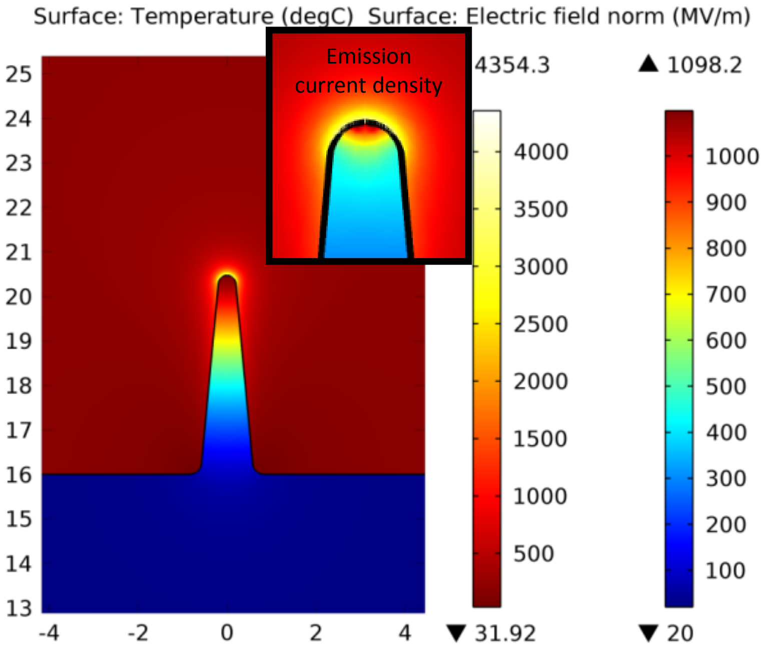
$$\langle \Delta E \rangle < 0 \rightarrow \text{heating}$$



$$\varphi_q = \langle \Delta E \rangle \frac{j(F,T)}{q}$$

# Heating and emission currents

## **Local** emission currents – connection to the experiment



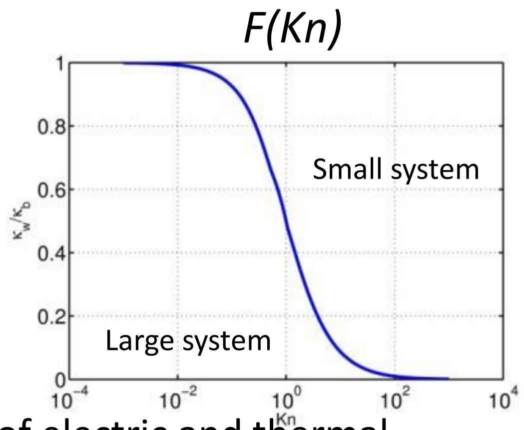
- Heat equation in steady state
- Fully coupled currents and temperature
- Emission currents concentrated to the top of the tip
- **Nottingham effect included in thermal modelling**

### Field emitters as nanowires

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

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

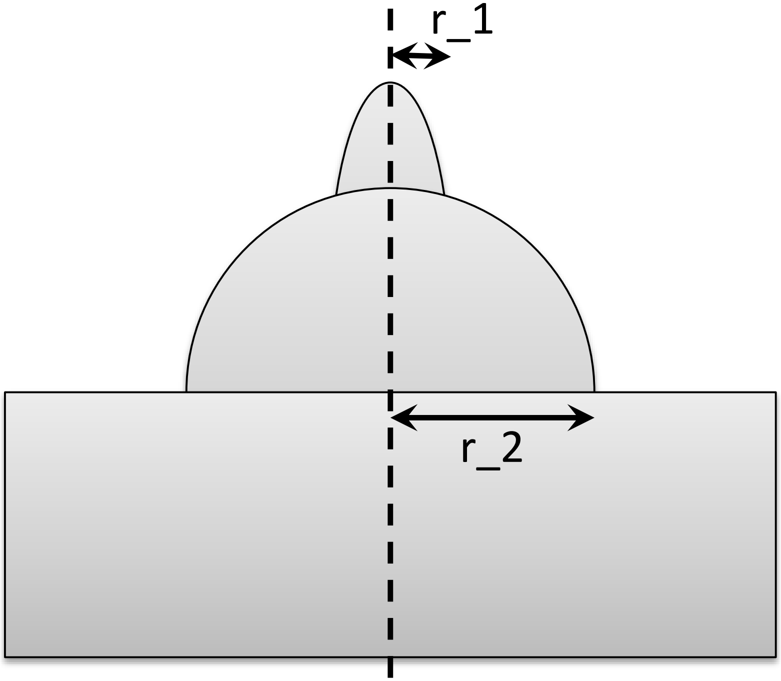
$$Kn = \frac{L_{free}}{d}$$



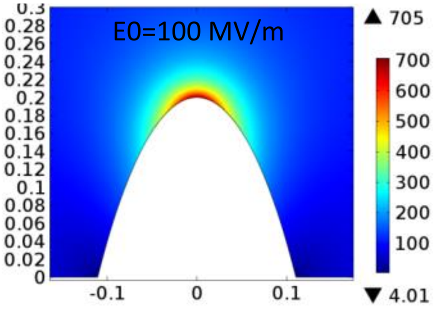
- Size dependence of electric and thermal conductivity
- Conductivity in nanoscale emitters is significantly decreased (more than 10x for sub-nanometer tip)
- Knudsen number to characterizes nanoscale size effects
- Wiedemann-Franz law for thermal conductivity
- **Optionally, temperature dependence in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

# Static behavior of single emitter – sensitivity to surface roughness

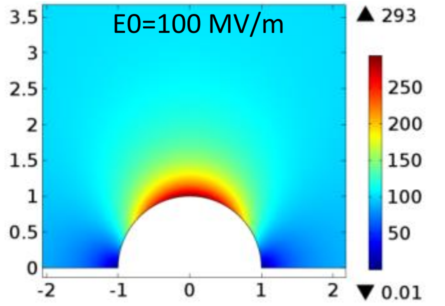
- We can see different surface modifications leading to small β
  - Large β is needed
- Multiplication of field enhancement factors
  - Can explain observed high beta values
- Incorporates surface roughness
- r_1/r_2<0.1 is needed to observe significant influence



Max. enhancement



Reference sim.

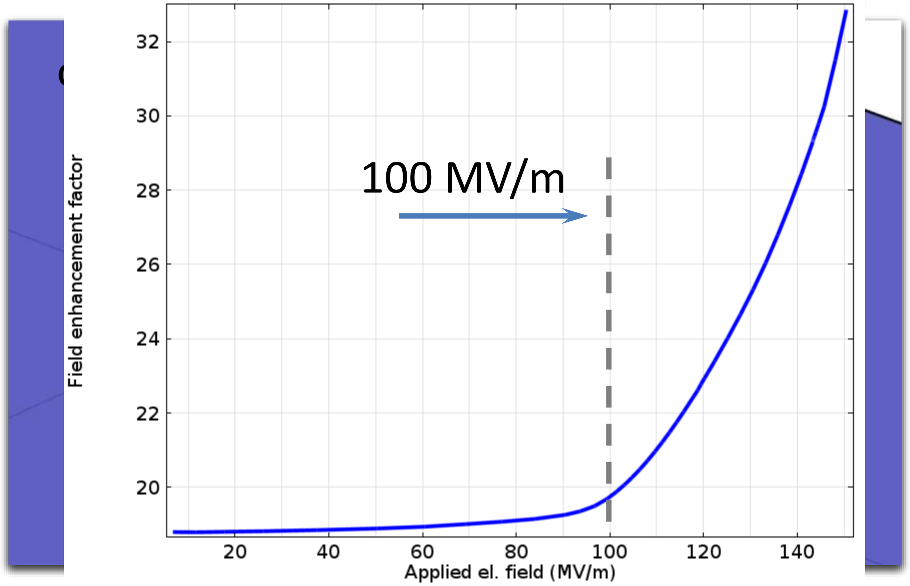


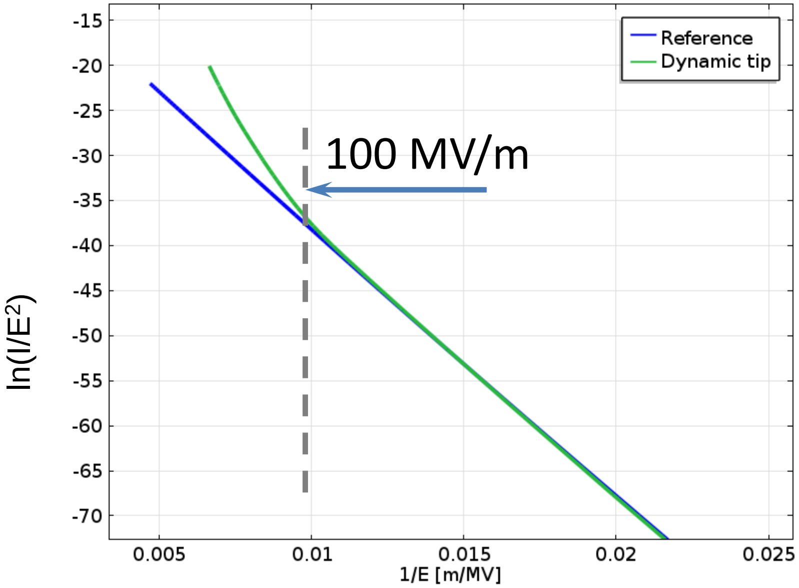
# Influence of dynamic surface modification

- Comparison of static (reference) and dynamic emitters
  - Static emitter does not change the shape during simulation
  - Dynamic emitter deforms elastoplastically

$\gamma$ - slope

$$\boxed{\beta = \frac{6.53x10^{3} \cdot \phi^{3/2}}{\gamma}}$$



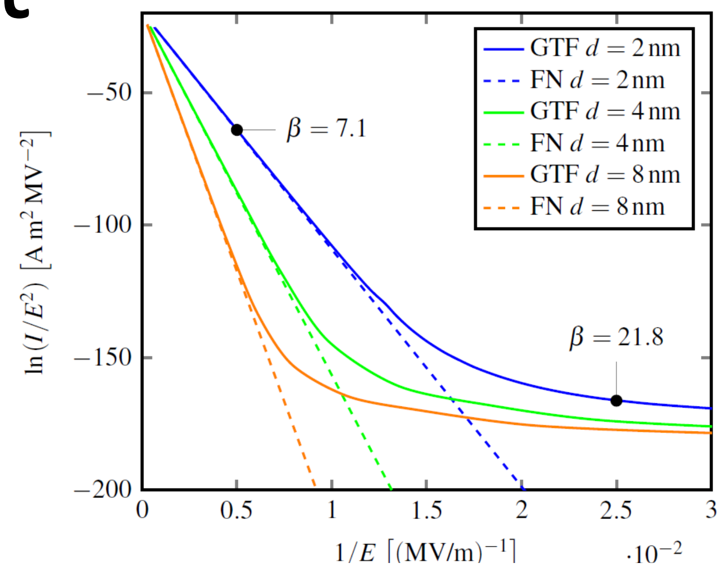


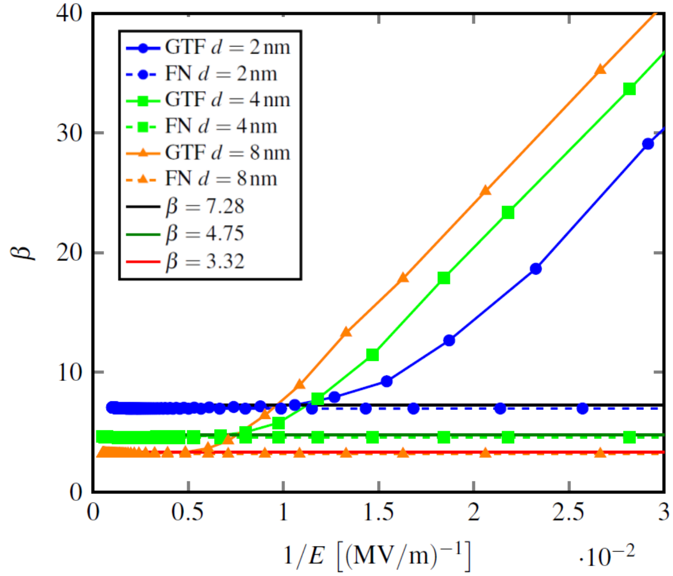
| | Direct calculation from simulation | From FN plot |
|---|---|---|
| Beta from static tip | 18 | 22 |
| Beta from dynamic tip | 18-33 | 11.5 |

- Beta decreases 2-3 times during dynamic deformation of emitter
- Instead of growing emitters, we have decreasing emitters?
- Evaporation of surface protrusions?

# Influence of temperature – FN plot

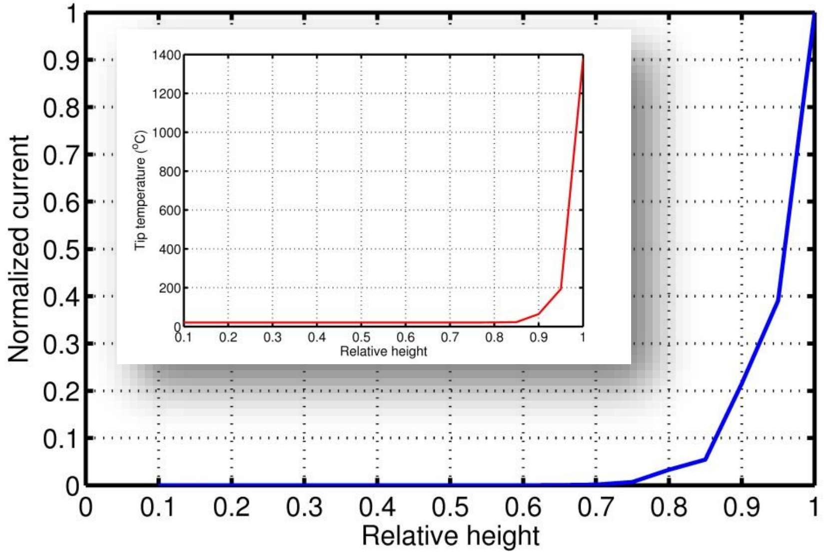
- Simulation of single emitter
  - Fully coupled currents, temperature and external field
  - Emission current is integrated over whole surface
- Taller emitters demonstrate smaller thermal effects
  - high local ***E*** is reached faster
  - Thermal effects influence lower applied fields
- FN equation assumes static system
  - Thermal effects introduce a dynamic component
- Problem – effect remains in low current region
- Possible use – allows us to estimate the actual size of the emitter?



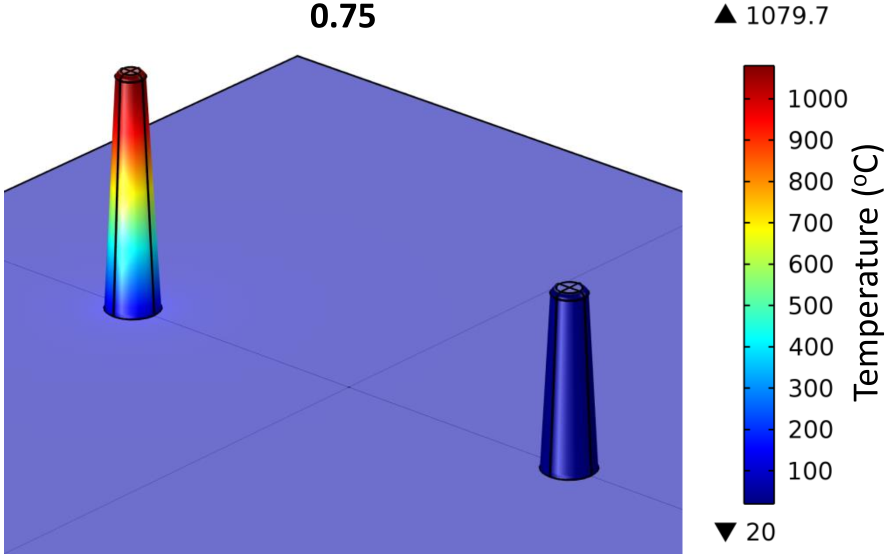


# Selective heating of the tips

- 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



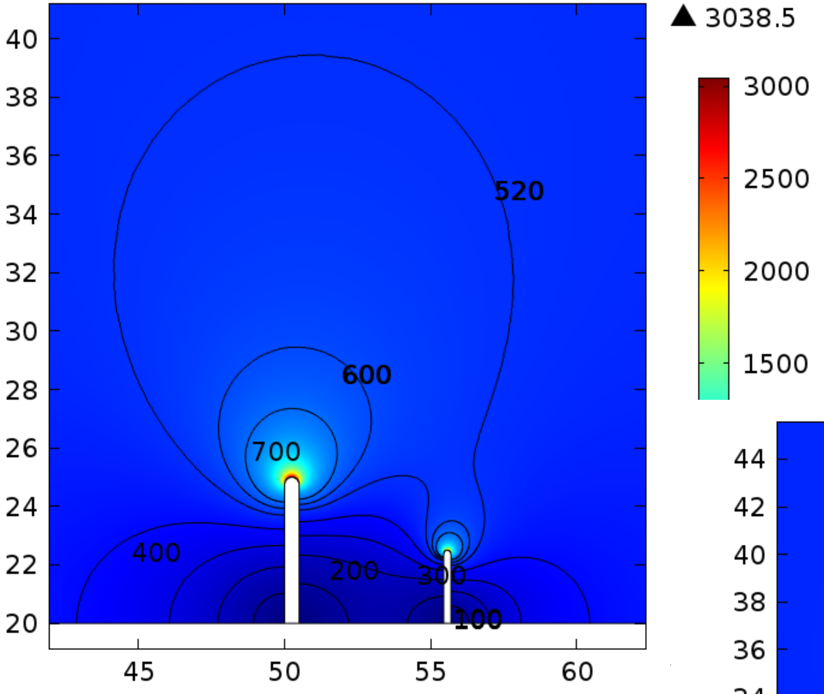
**Temperature of the tips, relative height 0.75**



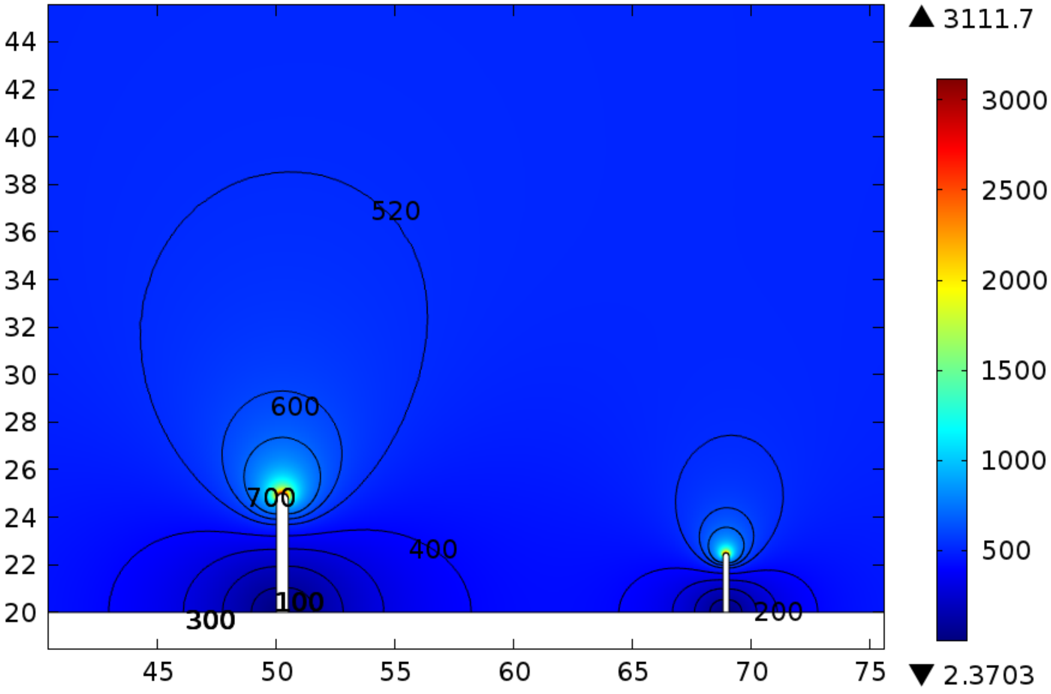
**Tip behavior under the el. field:**

- 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

# Electric field distribution due to interacting emitters



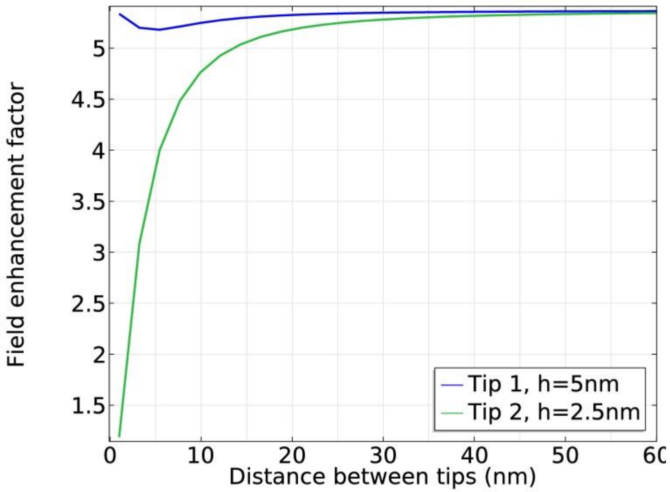
- Small emitter „captures“ part of the field from large emitter
- Smaller emitter is located in the low field region, created by tall emitter

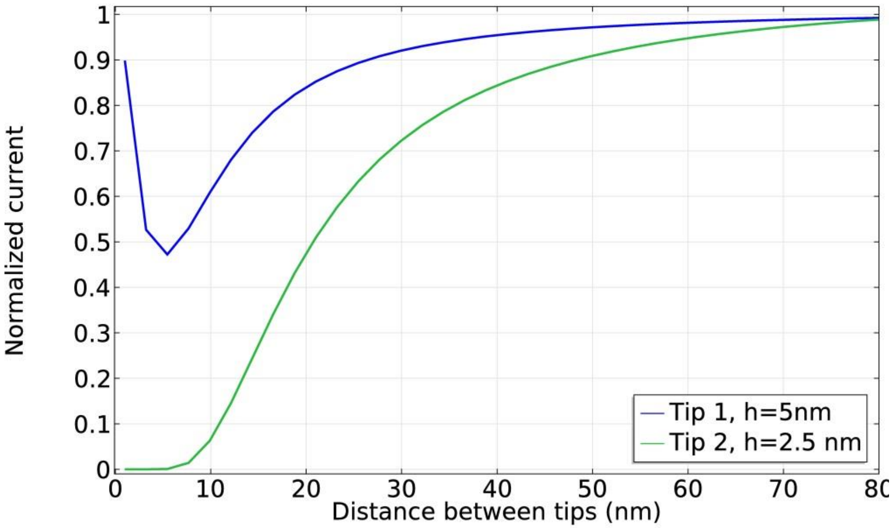


- Emission current sensitivity to the applied field
- **Local interactions on surface can have significant effect to the breakdowns**

# 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)

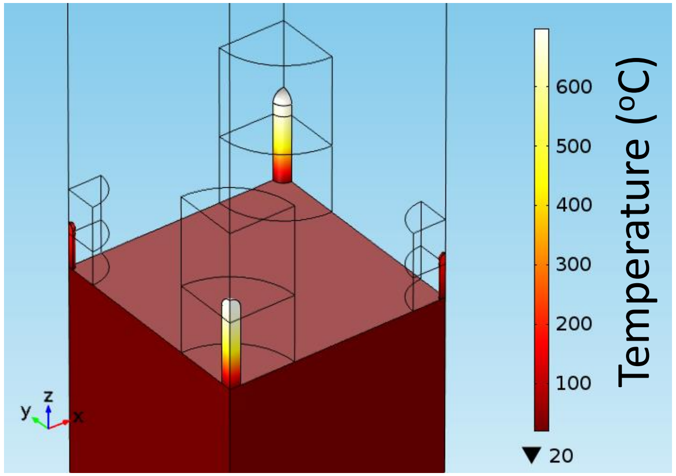


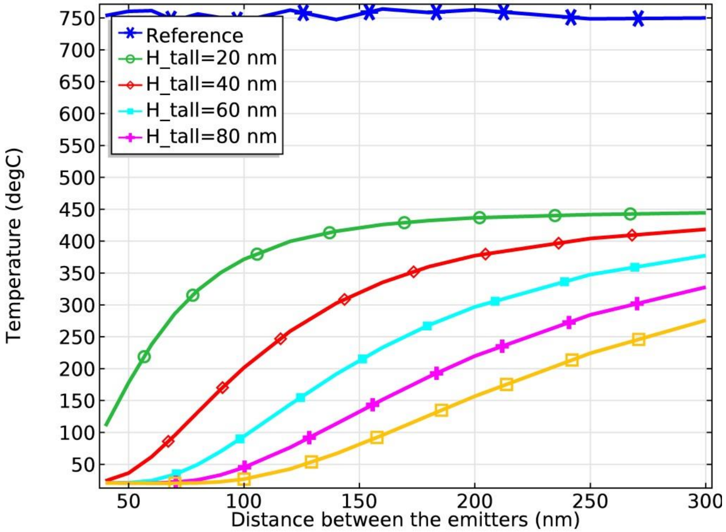


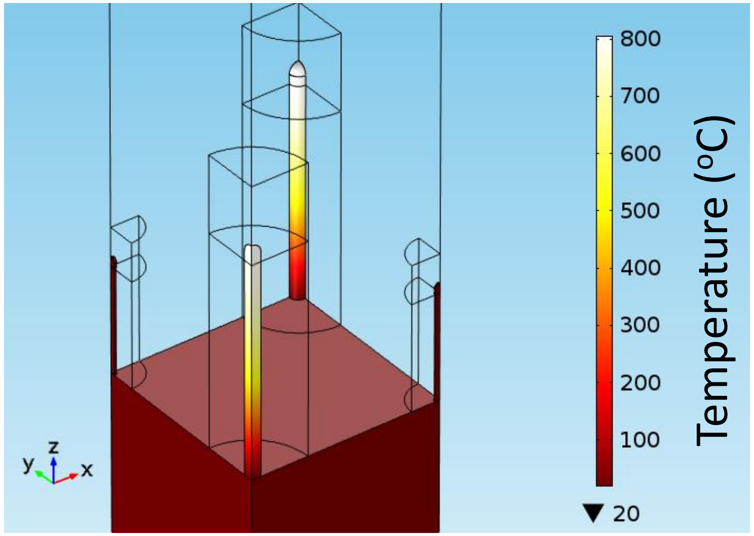
# Forest of emitters – the temperature distribution

In current figures scale=10

- H1=(2, 4, 6, 8) nm, H2=H1/2
- d1= 1 nm and d2=d1/2
- Distance 5 to 30
- Geometry scaling 1, 5,10 and 100
- Tall tip controls the emission currents
- If tall tip is destroyed, emission follows from equivalents smaller ones leading to consecutive breakdowns

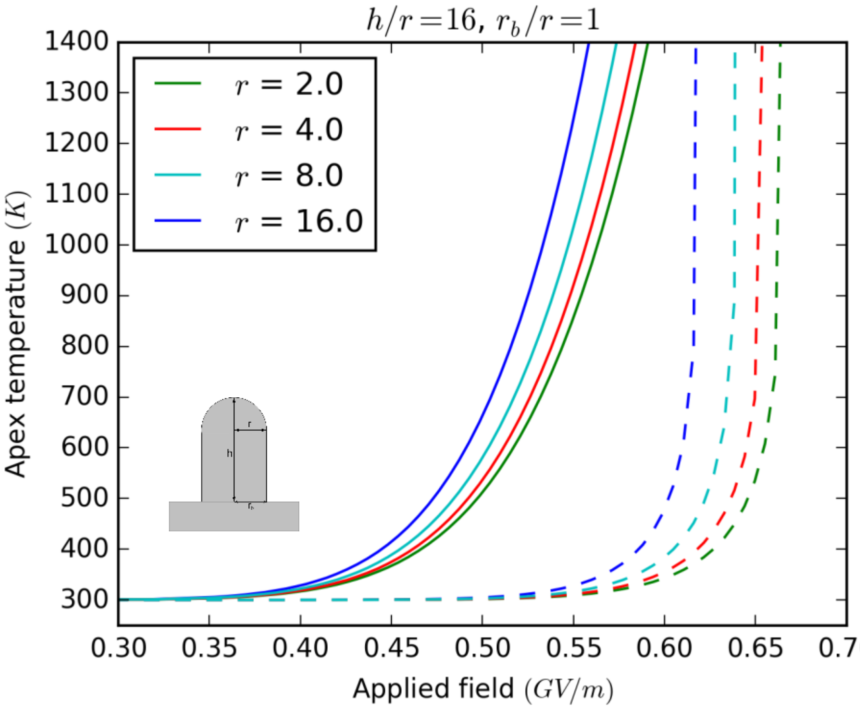






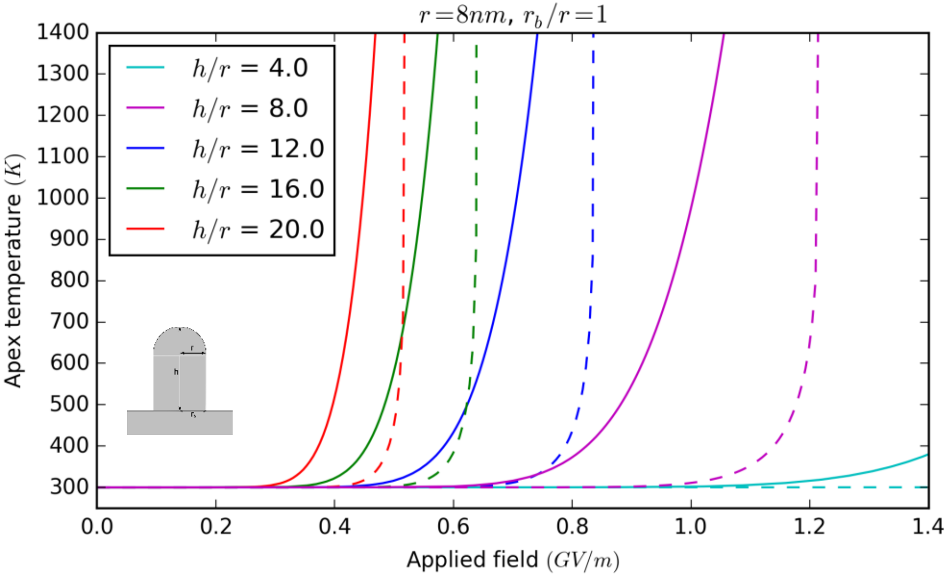
# Influence of Nottingham effect I

- Nottingham effect provides significant additional heating
- **Joule heating only provides a limiting case information**
- Smaller emitters can be melted
  - Reduces the cooling effects of bulk material



- Aspect ratio of emitter is constant
- Radius height is changing

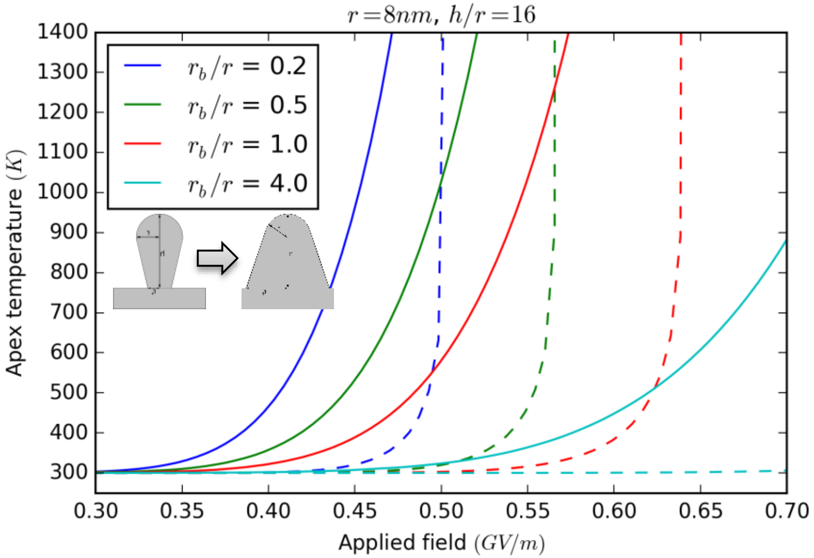
# Influence of Nottingham effect II



- Constant radius, variable height calculations

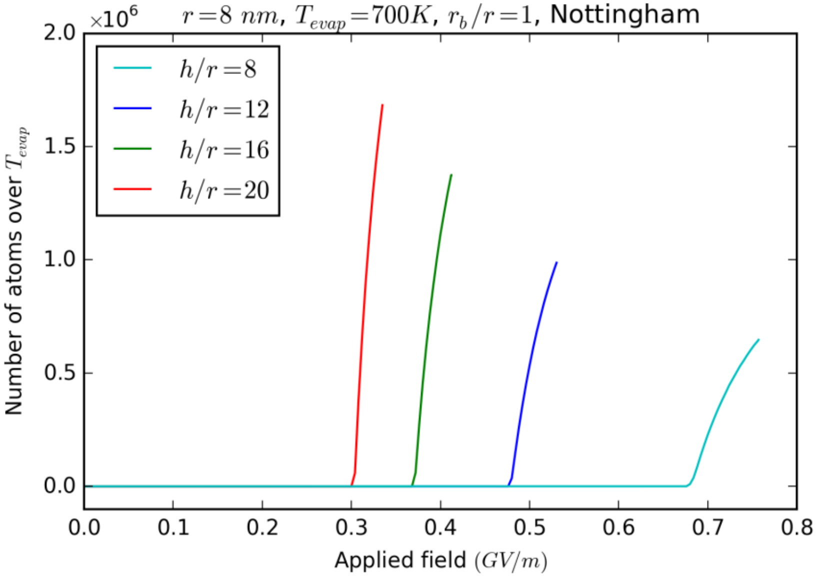
- Influence of the emitter shape – conical emitters vs. straight ones

**Ability to melt both, larger and smaller tips!**



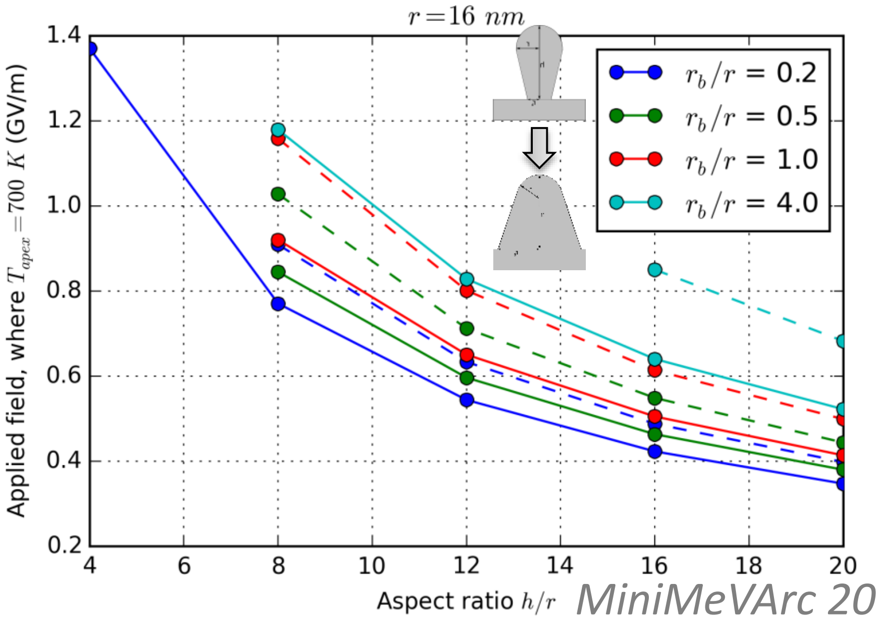
- Reduces aspect ratio of emitters that can be molten by applied fields
- Significant influence in case of conical emitters!
  - Conical, low aspect ratio emitters as possible sources of neutrals as well

# Evaporated atoms versus applied field

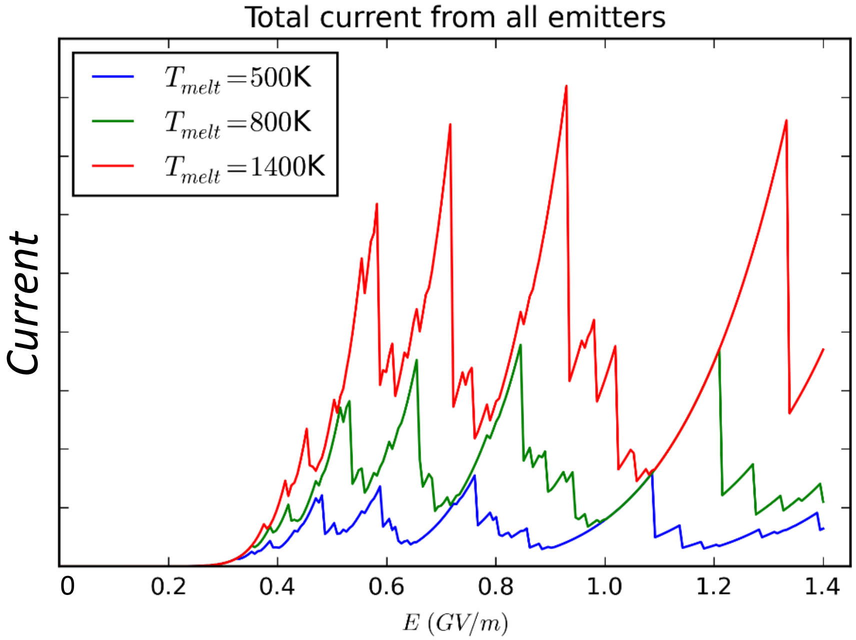


- Estimation of number of neutrals in vacuum based on emitter temperature
- Allows to detect size and number of emitters, needed for a BD

- Molten material estimated by integrating emitters volume with $T>T_{melt}$
- Melting temperature of nanoparticles has significant size dependence



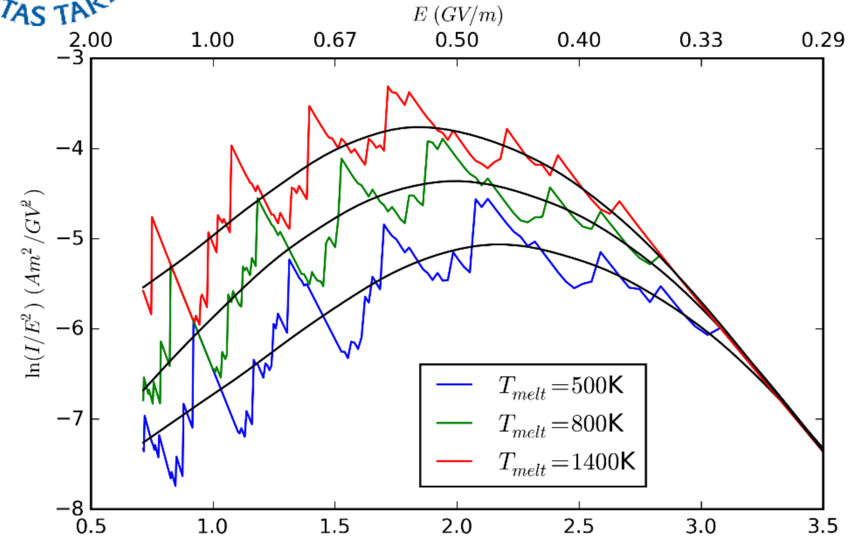
# Combined current from all emitters

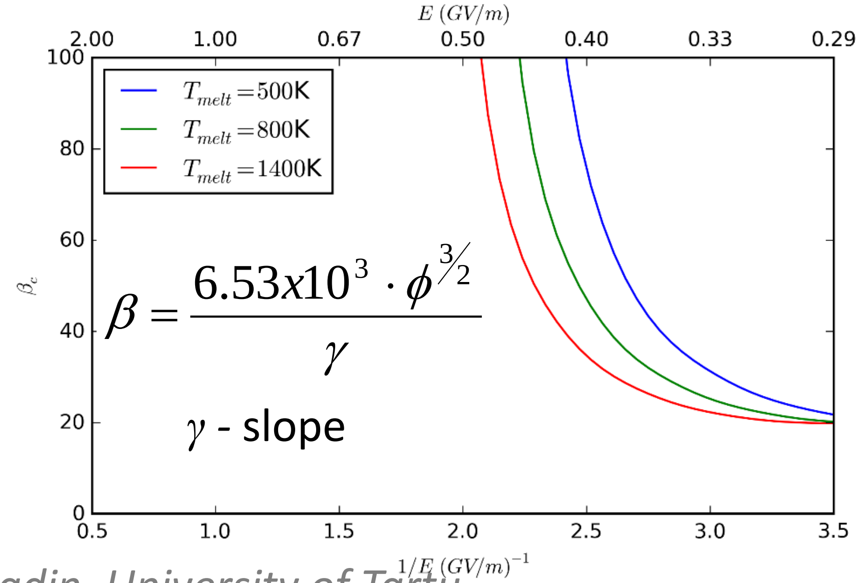


Based on integrated current and corresponding el. field range, Fowler-Nordheim plot is constructed

- Currents from all emitters are added
- Only one emitter is considered from each geometrical configuration
- Interactions between the emitters are not considered
- **Current from emitter stops, if melting temperature is reached**

# Influence to the field enhancement factor





$$\beta = \frac{6.53x10^3 \cdot \phi^{3/2}}{\gamma}$$

$\gamma$ - slope

- Dynamic effects of surface change due to the melting of emitters
- Current calculations assume 1 emitter from each set of geometrical parameters
  - Some geometries may be unphysical
  - More emitters than 1 from different types may be present
  - **Statistical distribution is needed for different emitters!**
- Statistics of the emitter types can be obtained by using data fitting with optimization methods (genetic algorithms)
  - Comparison with emission current measurements
  - Comparison with breakdown rate measurements
  - Comparison with stochastic breakdown estimation models

# Conclusions

- FEM is viable and flexible tool for studying surface modification phenomena
- Nottingham effect provides significant additional heating
- Dynamic behavior of surface due to the melting of emitters has capacity to influence the field enhancement factor

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