Compact Linear Collider: Investigation of electrical breakdown phenomena using multiscale and multiphysics simulations

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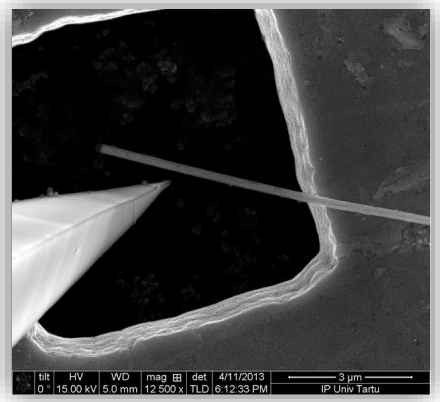
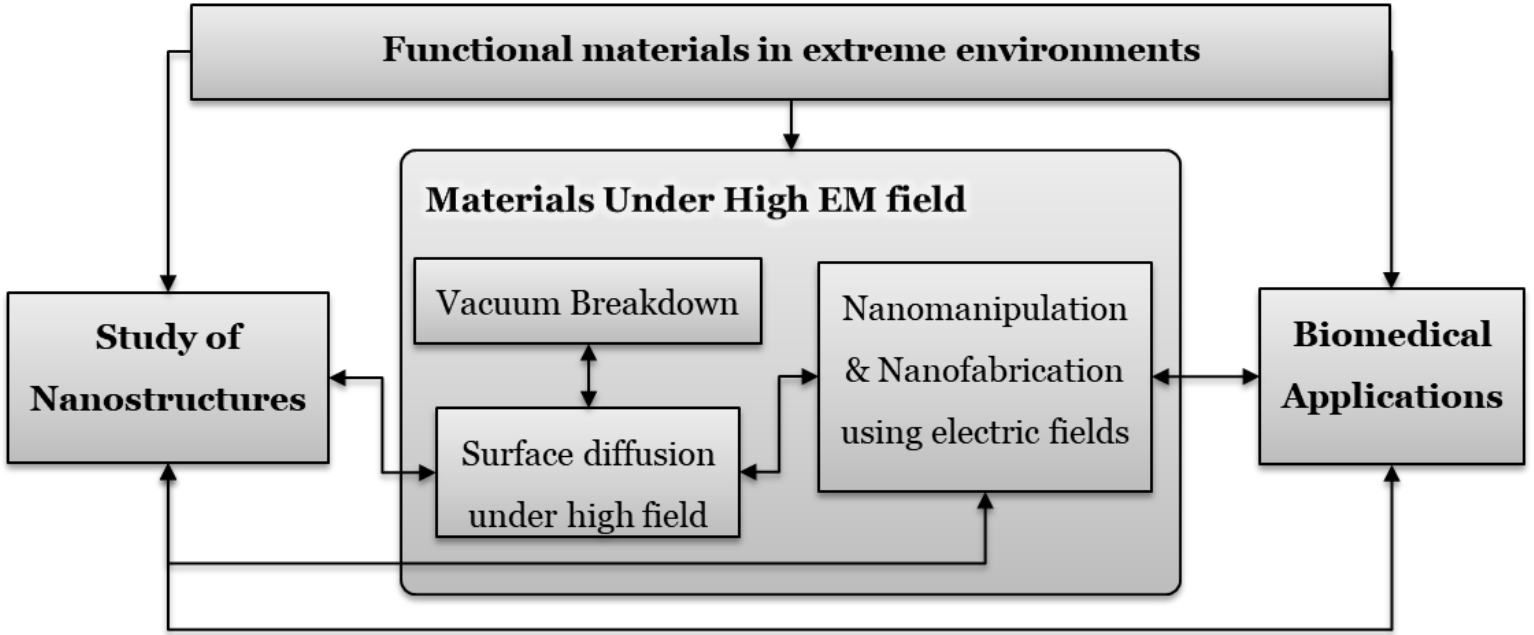
CBC 2022

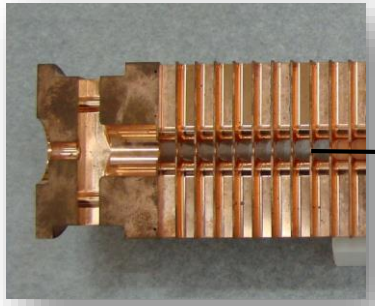
University of Tartu: ERA Chair MATTER

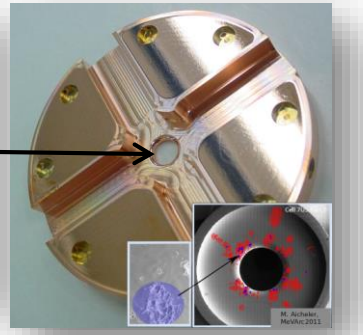


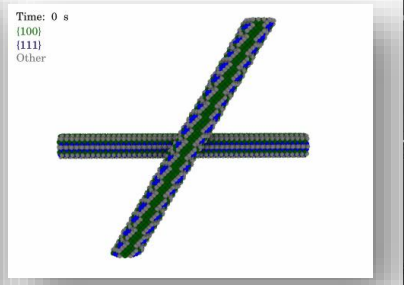
Essential tools

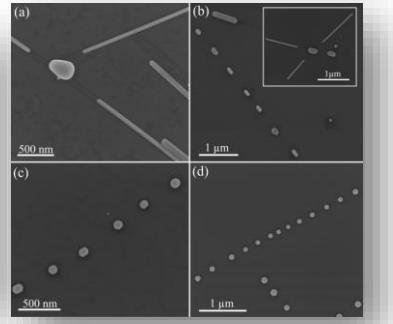
- Multi-scale simulations
- In-situ Nanomanipulation
- SEM, TEM, AFM

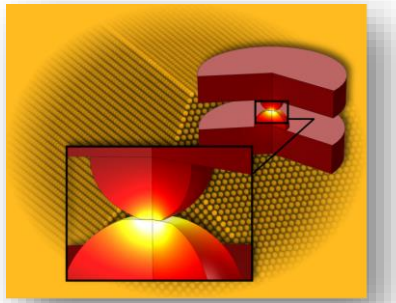


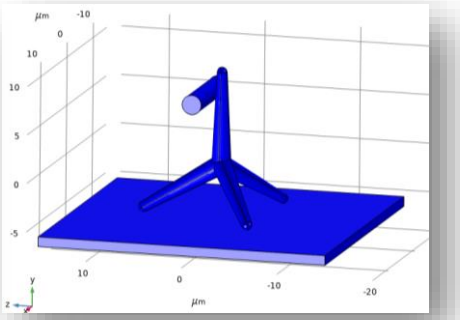












ERA Chair MATTER: Team in action

- **Veronika Zadin**, PhD, prof., coordinator, advanced computer simulations
- **Andreas Kyritsakis**, PhD, ERA Chair holder, associate prof., advanced computer simulations
- **Sergei Vlassov**, PhD, associate prof., Nanomanipulation team lead
- **Veikko Linkko** , PhD, associate prof., Biomedical team lead
- **Sven Oras**, PhD, Postdoc
- **Edgars Butanovs**, PhD, Postdoc
- **Tauno Tiirats**, PhD, Postdoc
- **Mihkel Veske**, PhD, engineer
- **Mart Ernits**, MSc, PhD student
- **Ye Wang**, MSc, PhD student
- **Elyad Darmechi**, MSC, PhD student
- **Roni Koitermaa**, MSC, PhD student
- **Mikael Rinne**, Engineer, BSc student
- **Theophilus Odubena**, BSc student
- **Ihar Suvorau**, BSc student
- **Kristi Koitla**, BSc student
- **Margit Meiesaar**, supporting staff

CLIC – Compact Linear Collider in https://clic.cern/

MATTER

Applicat
- **CLIC**
- vacu
- nove
- x-ray
- medi
- RF co

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devices

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res E ~ 100 MV/m

→ BD

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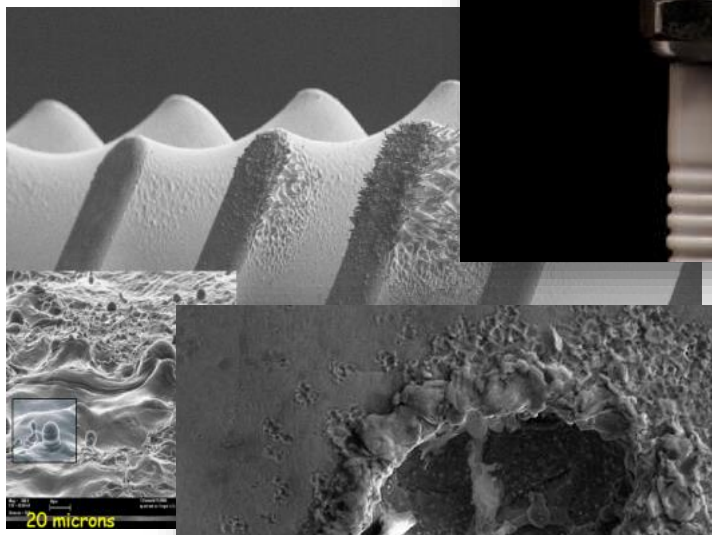
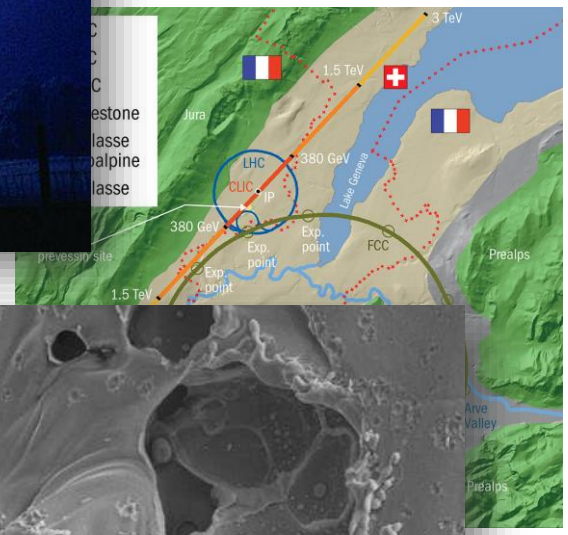
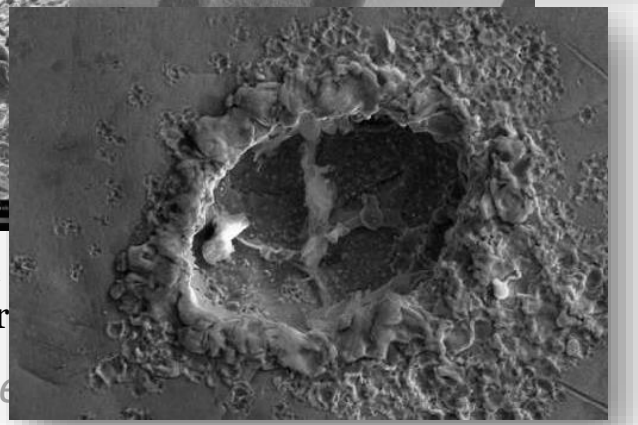
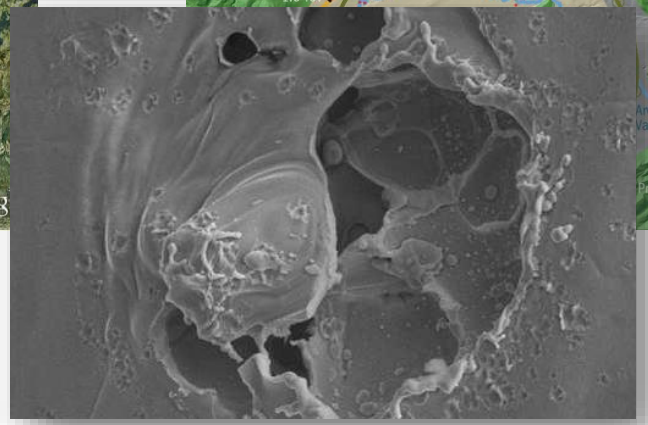


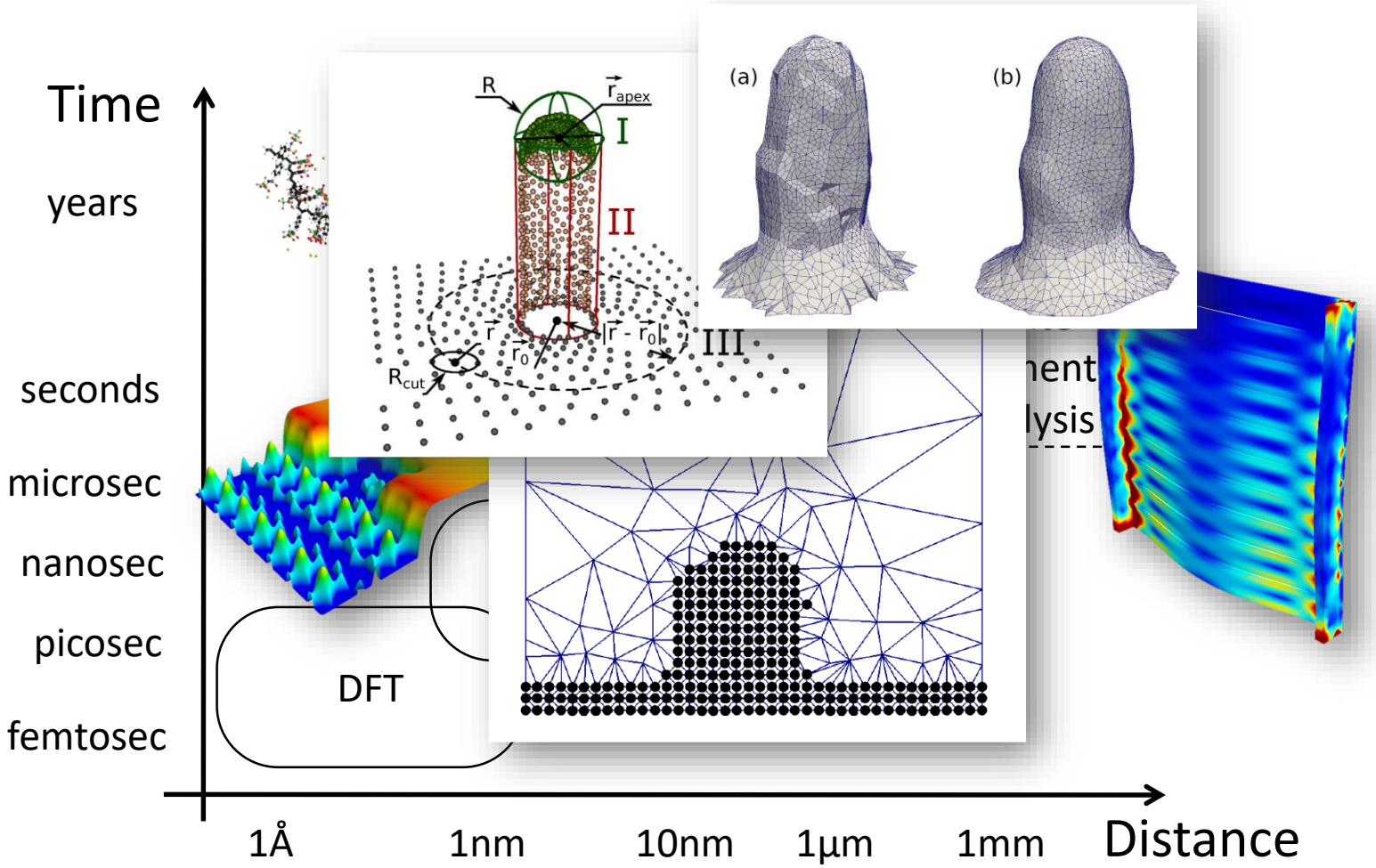






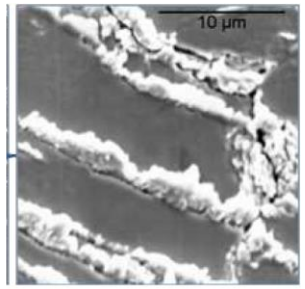
Surface
structur

How we decode the nature …

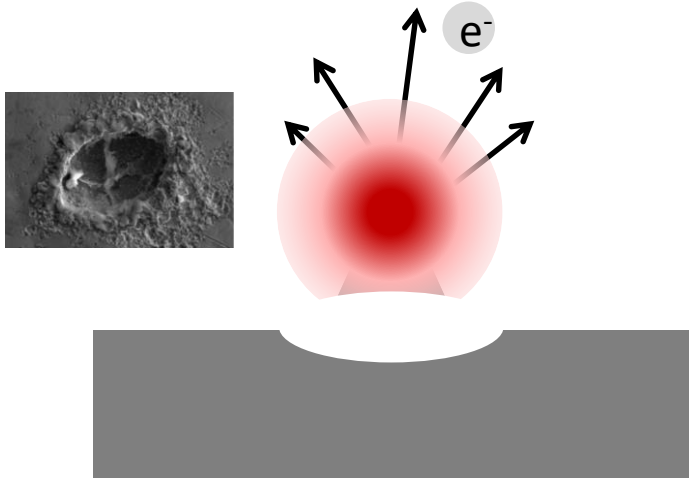


Breakdown initiation mechanisms

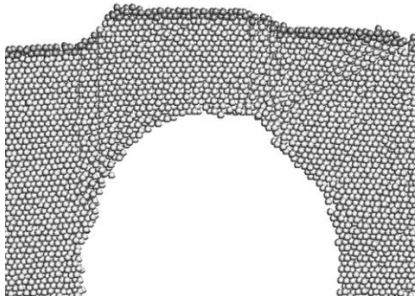
Fatique damage



L. Laurent *et al.*,
Phys. Rev. ST Accel. Beams. 14 (2011)



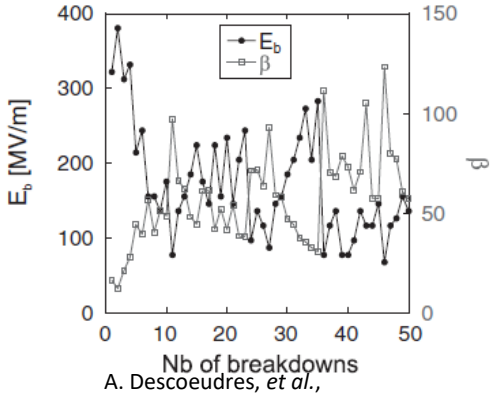
Subsurface defects



A. Pohjonen, F. Djurabekova, et al.
*J. Appl. Phys. (*2013)

Emission current measurements
Field enhancement factor β

Key problem 1:
understanding the mechanism leading to the appearnce of the field emitter



A. Descoeudres, *et al.*,
Phys. Rev. ST Accel. Beams. 12 (2009)

Key problem 2:
understanding actual formation of field enhancement factor ~100

Field emitters with height to radius ratio ~100 (100 nm tall with 1 nm diameter) needed????

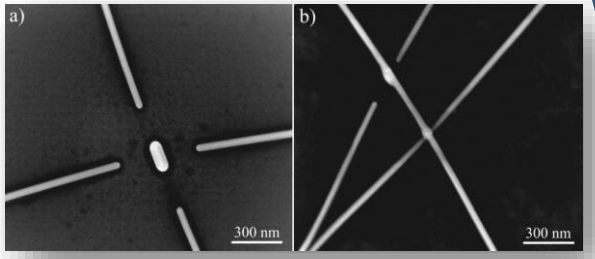
Unlocking BD onset

KIMOCS
Gold model systems,
Surface behaviour

MD, DFT, FEMOCS, GETELEC
Surface stability, estimation of possible phenomena

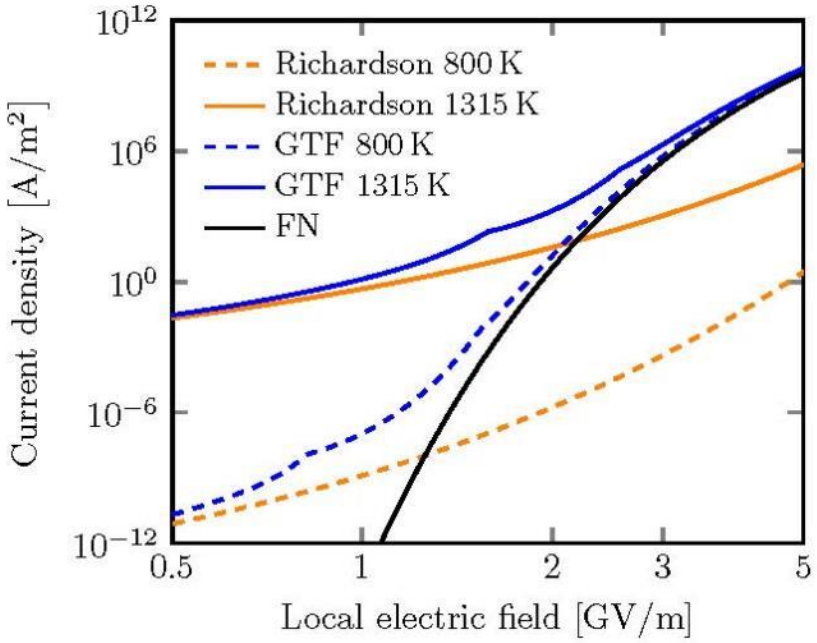
In situ SEM:
- Heating & diffusion
- Local El. field

FEM modeling,
Upscaling in *X* and *t*
Expectations of experimental conditions



The emission currents & thermal effects of electron emission

Electron Emission by General Thermal Field model



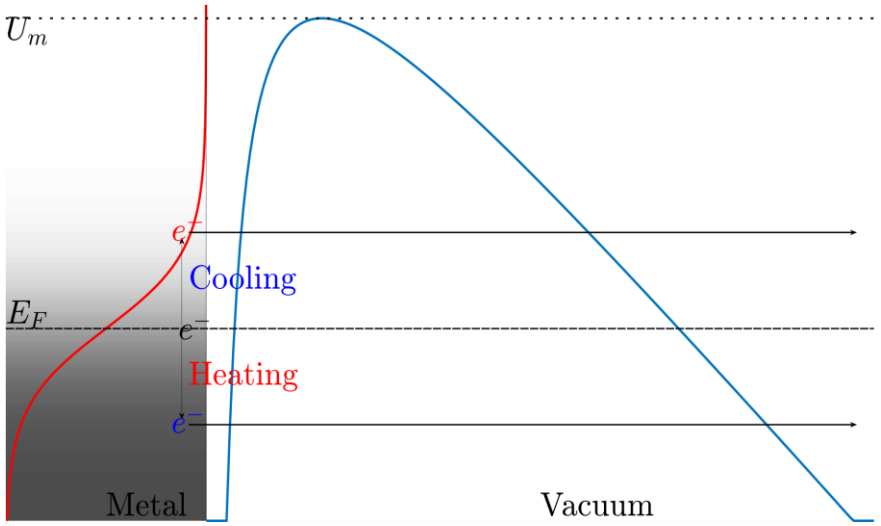
- Thermionic emission: high temperature, low field
- Field emission: low temperature, high field
- Combined effects: general thermal field equation

Two heat deposition components

- Joule heating $P_J = J^2/\sigma$ (volumetric heat deposition)
- Nottingham heat (surface heat deposition)

$$P_N(F,T) = \int \left(E(\vec{k}) - E_F\right) f_{FD}(\vec{k};T) D(\vec{k}) d^3k$$

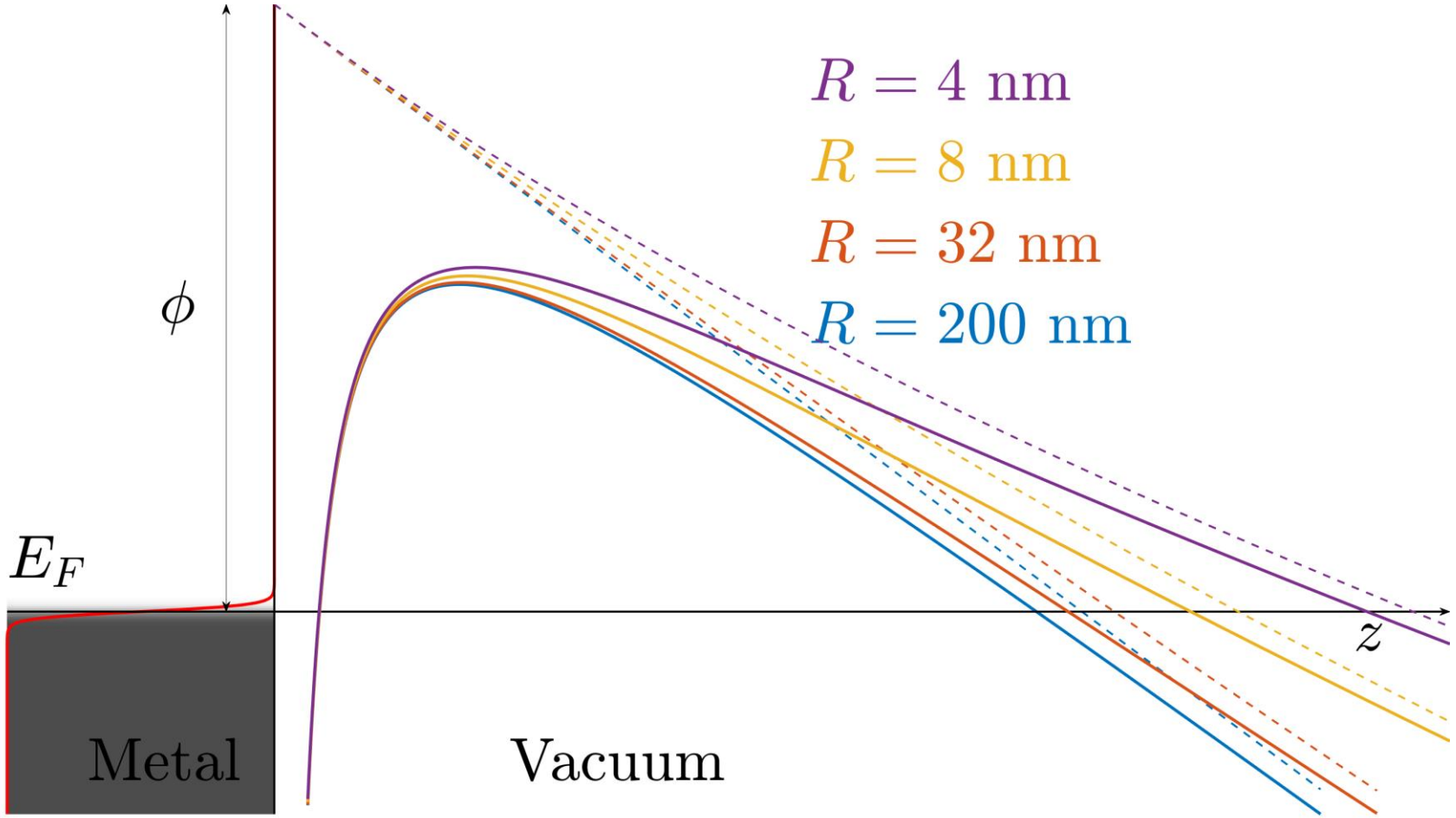
$$= J_s \langle E - E_F \rangle / e$$



Electron emission and heating by GETELEC Code: https://github.com/AndKyr/GETELEC

A. Kyritsakis, F. Djurabekova, Comput. Mater. Sci 128 15 (2017)

Sharp emitter effects



- General barrier formula:

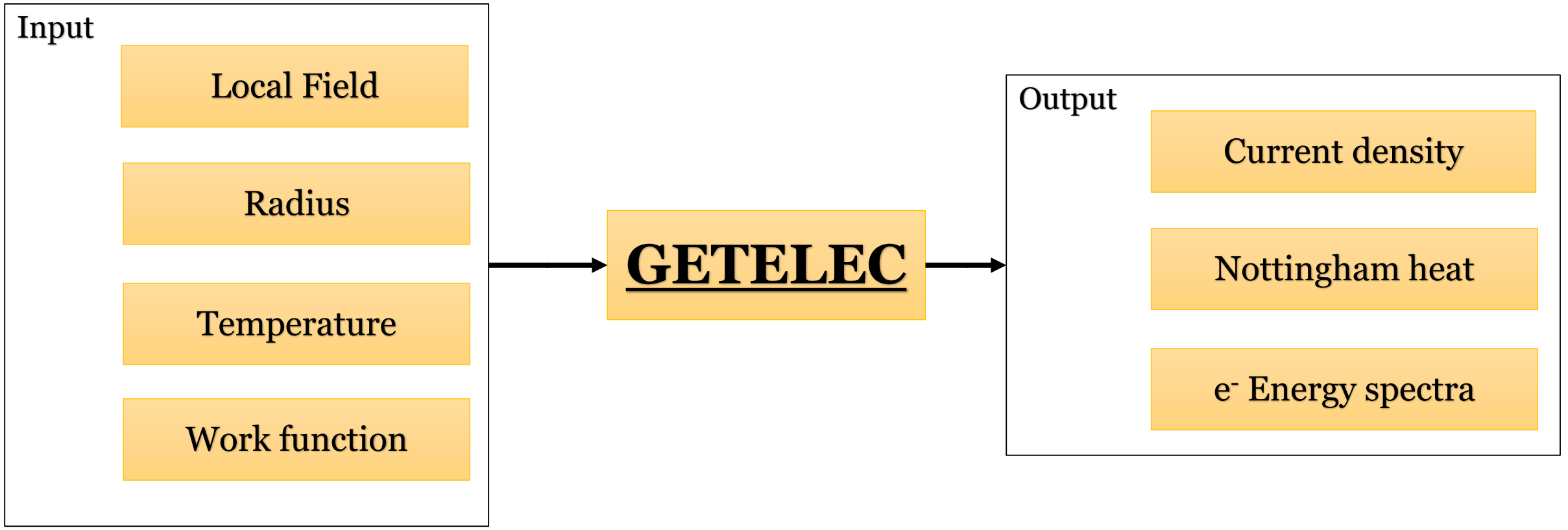
$$\Phi(x; F, R, \gamma) = F\frac{R(\gamma-1)x + x^2}{\gamma x + R(\gamma-1)}$$

$$F = \left[\frac{d\Phi}{dx}\right]_{x=0}$$

$$R = -\frac{2F}{\left[\frac{d^2\Phi}{dx^2}\right]_{x=0}}$$

$$\gamma = \frac{F}{\left[\frac{d\Phi}{dx}\right]_{x=\infty}}$$

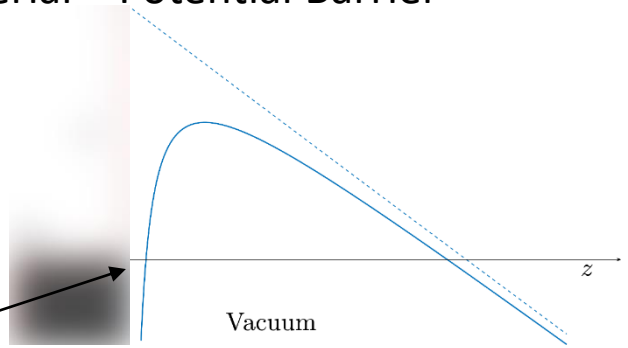
GETELEC



- More details: A. Kyritsakis et. al., Comput. Meter. Sci. 128, 15–21 (2017)

Code implementation

Material + Potential Barrier



Later retrieve by interpolation

Input

Pre-calculated

Local Field

Radius

Temperature

Band structure

Nested self-consistent

GETELEC

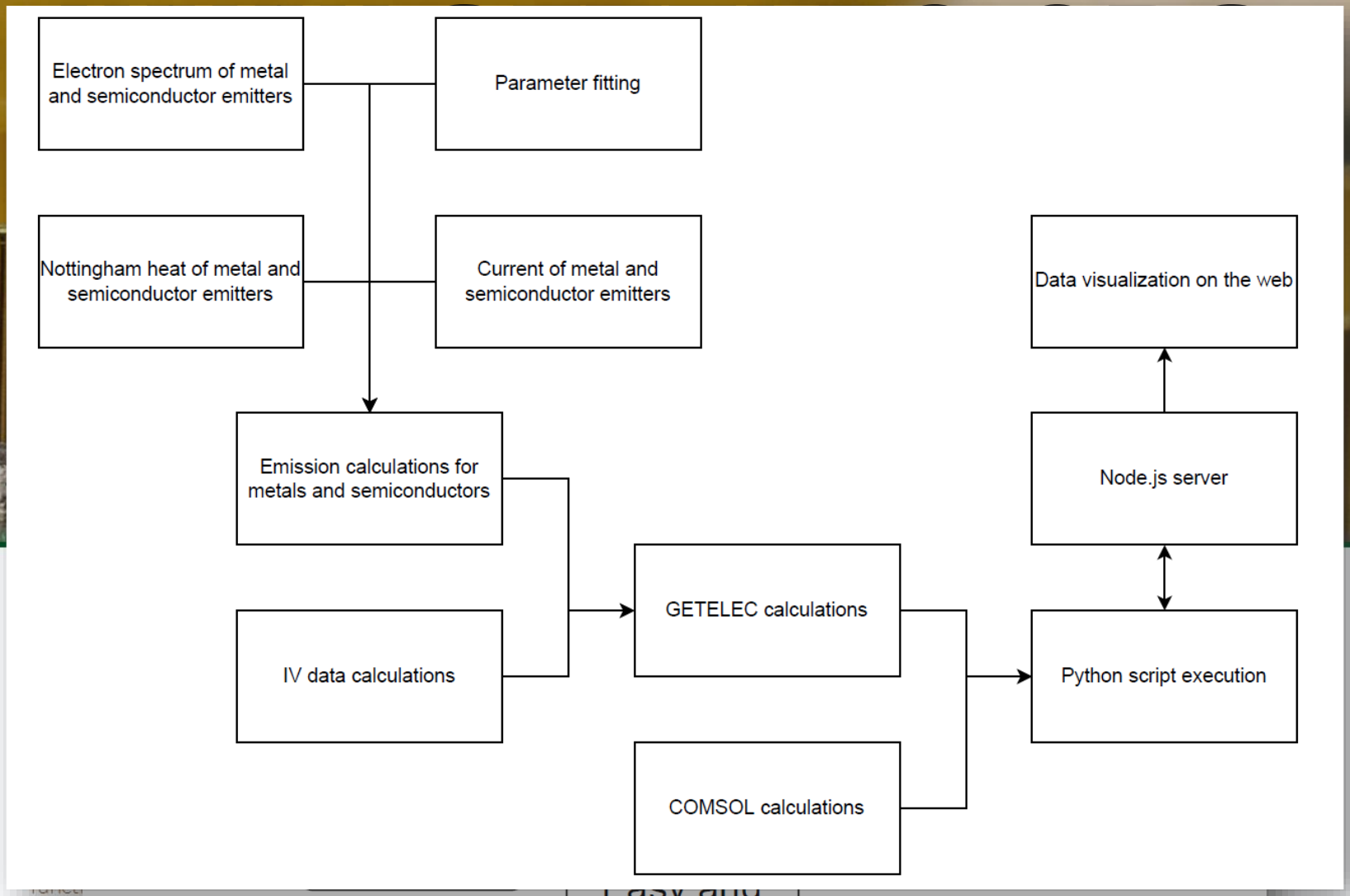
No analytical solutions for our integrals!

Output

Current density

Nottingham heat

e^- Energy spectra

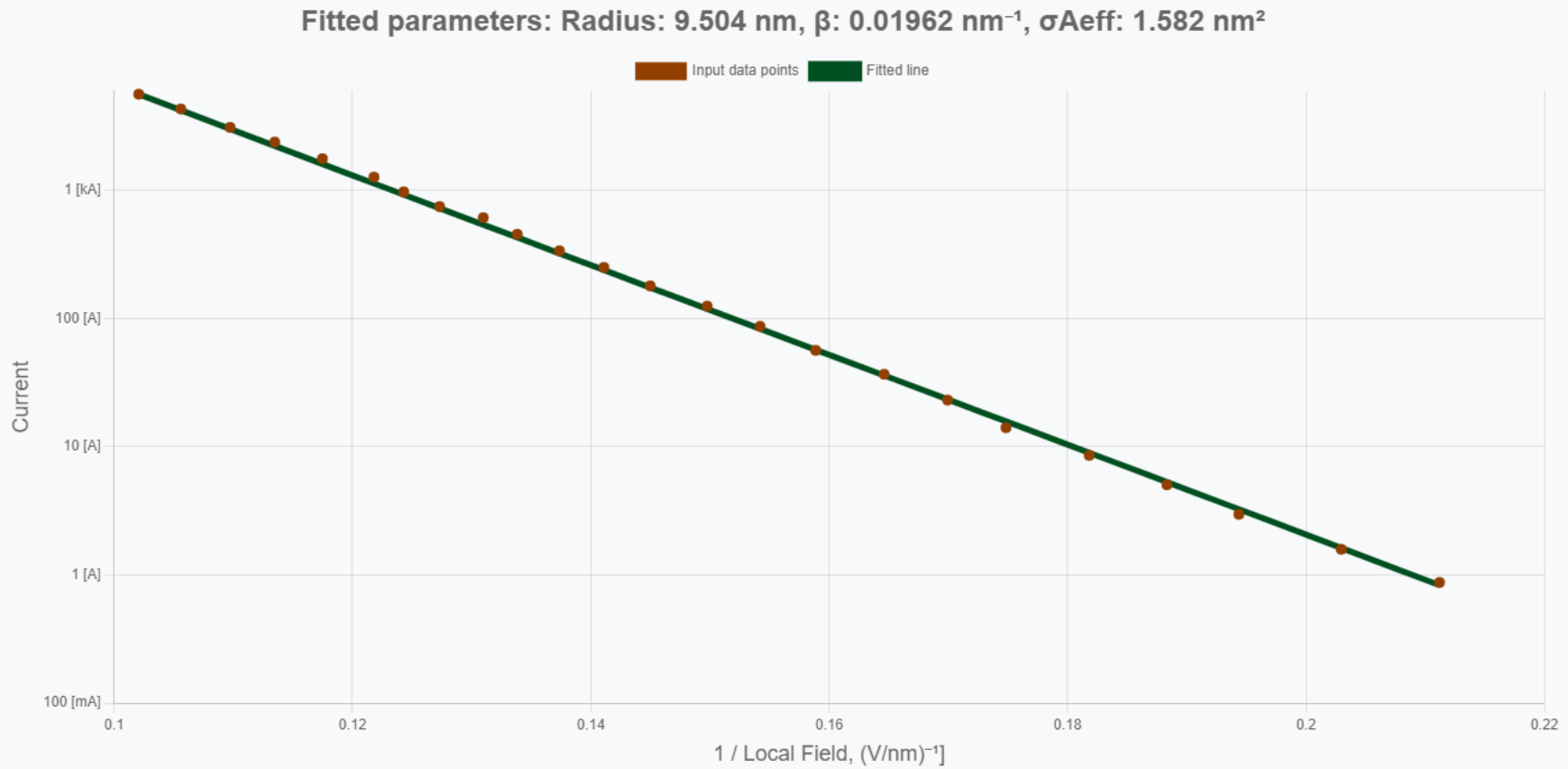


Easy and quick setup

GETELEC

Voltage	2.413e+02, 2.511e+02, 2.622e+02, 2.706e+02, 2.803e+02, 2.915e+02, 2.999e+02, 3.096e+02, 3.208e+02, 3.305e+02, 3.403e+02, 3.515e+02, 3.	[V]
Current	8.719e-01, 1.582e+00, 2.967e+00, 5.038e+00, 8.555e+00, 1.406e+01, 2.309e+01, 3.670e+01, 5.643e+01, 8.678e+01, 1.249e+02, 1.797e+02, 2.!	[A]
Work Function	4.5	[eV] Enter

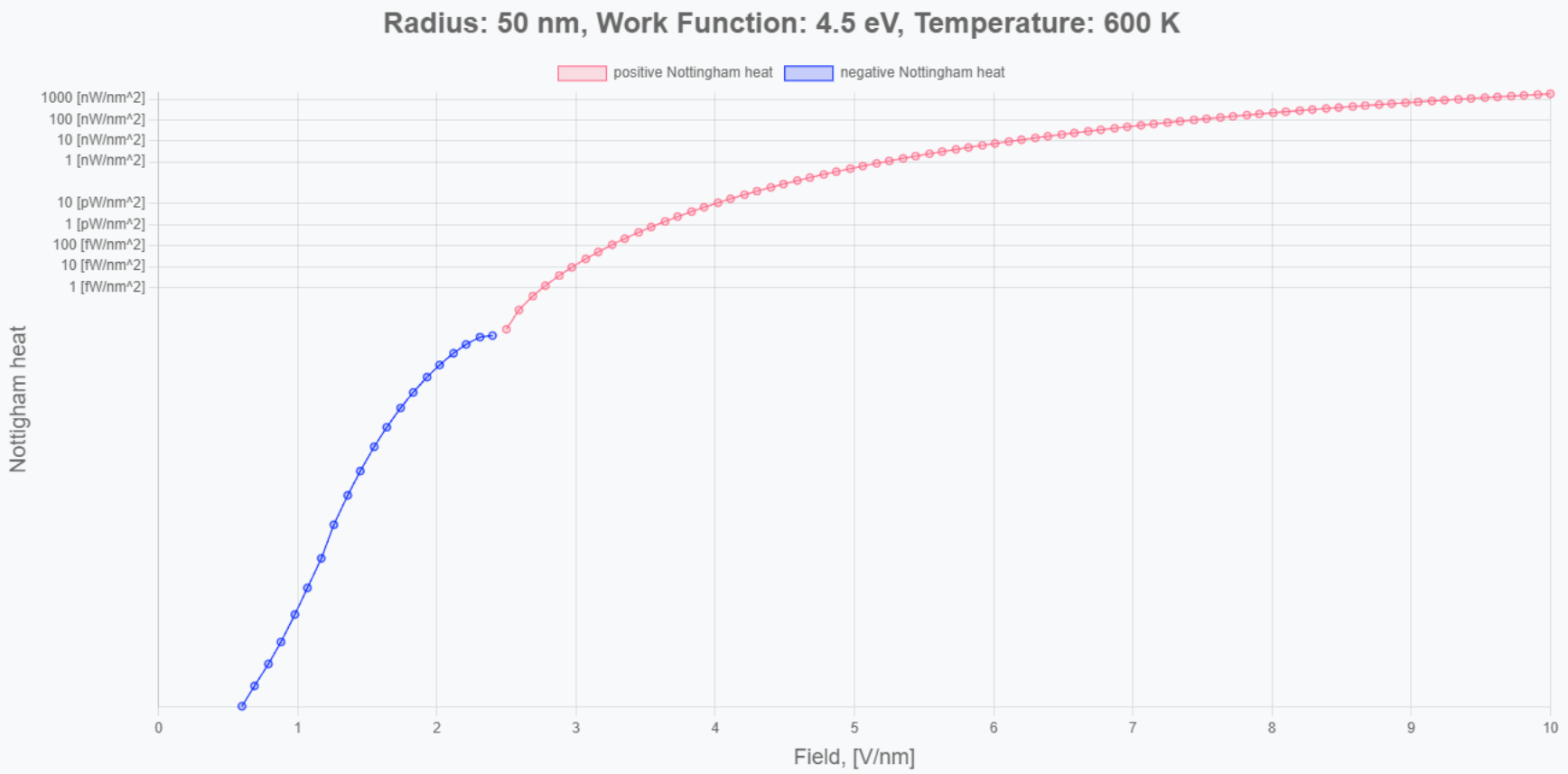
2



Download data

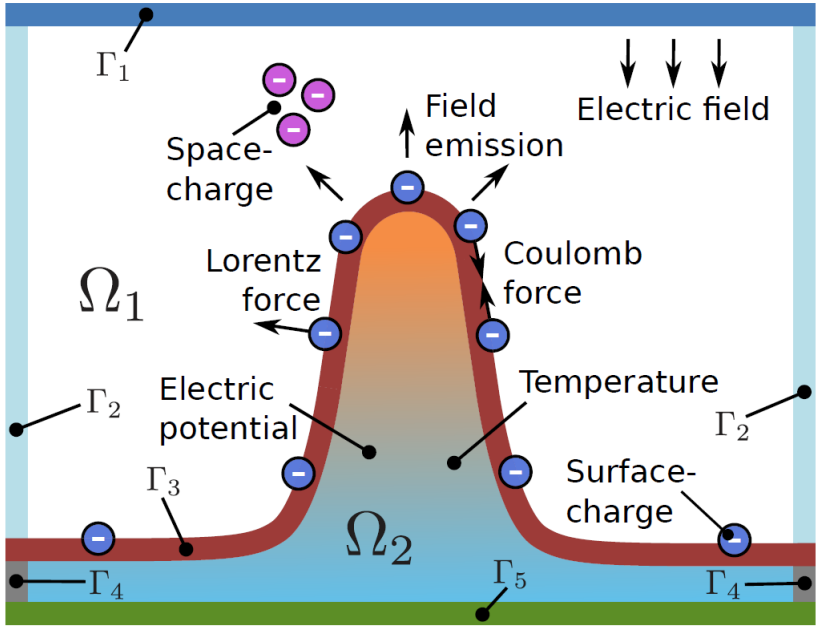
How to use

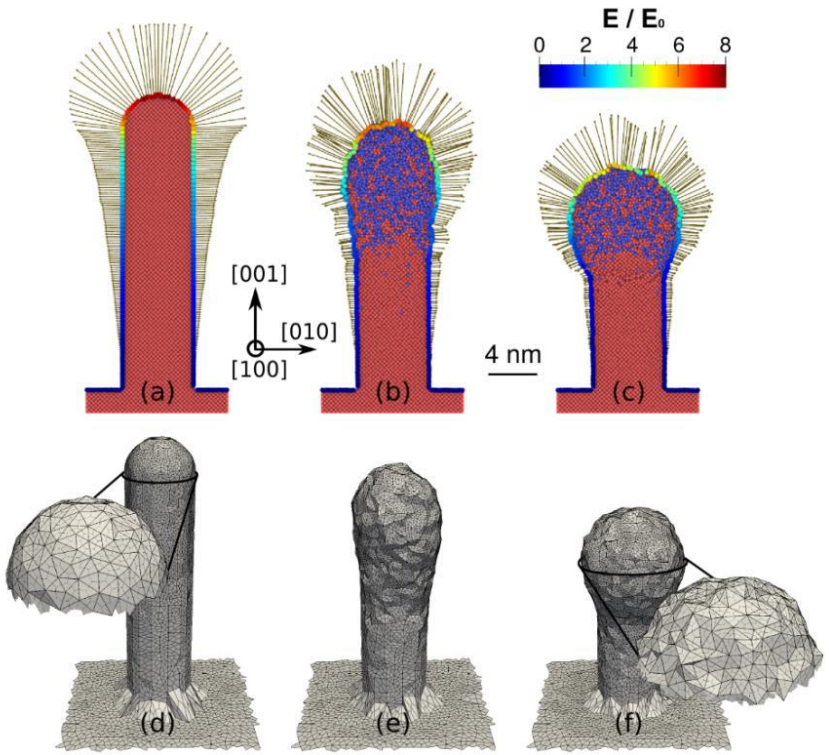

0
1
2
3
4
5
6
7
8
9
10
Field, [V/nm]

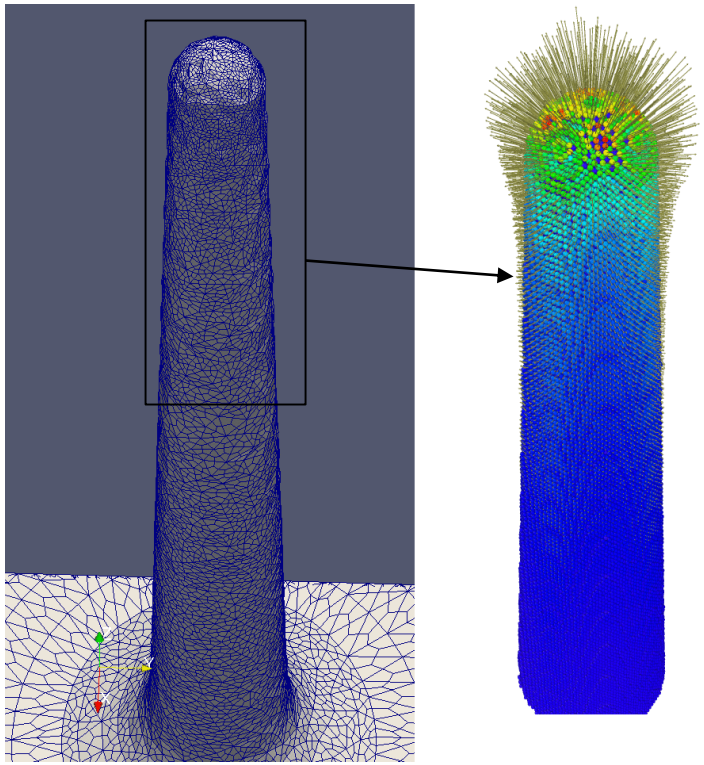

Radius: 50 nm, Work Function: 4.5 eV, Temperature: 600 K
positive Nottingham heat
negative Nottingham heat
1000 [nW/nm^2]
100 [nW/nm^2]
10 [nW/nm^2]
1 [nW/nm^2]
10 [pW/nm^2]
1 [pW/nm^2]
100 [fW/nm^2]
10 [fW/nm^2]
1 [fW/nm^2]
Nottigham heat
0
1
2
3
4
5
6
7
8
9
10
Field, [V/nm]


electron spectrum
1.0
0.9

Concurrent ED-MD: FEMOCS







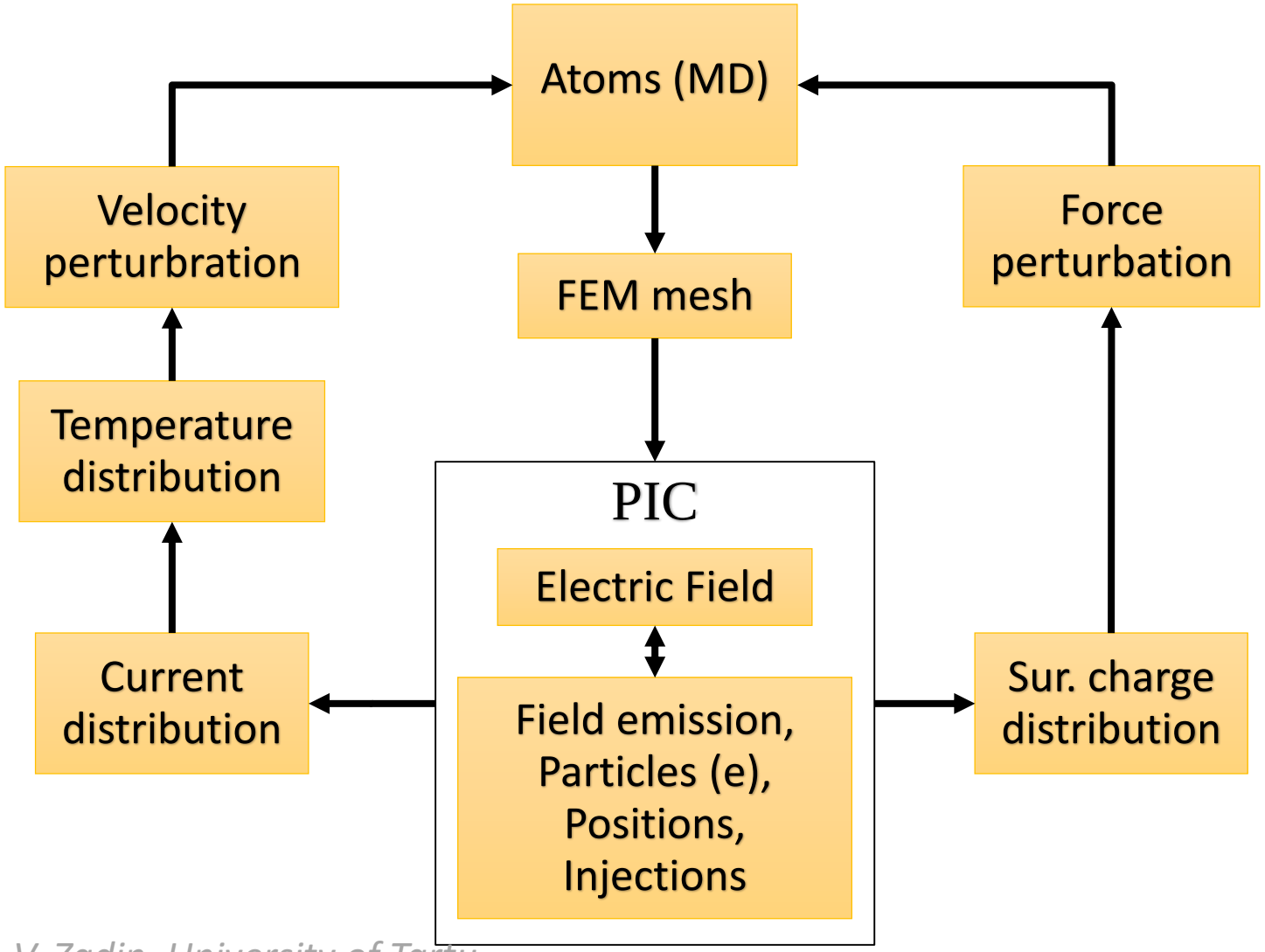
Fine elements:
- Deal.II library

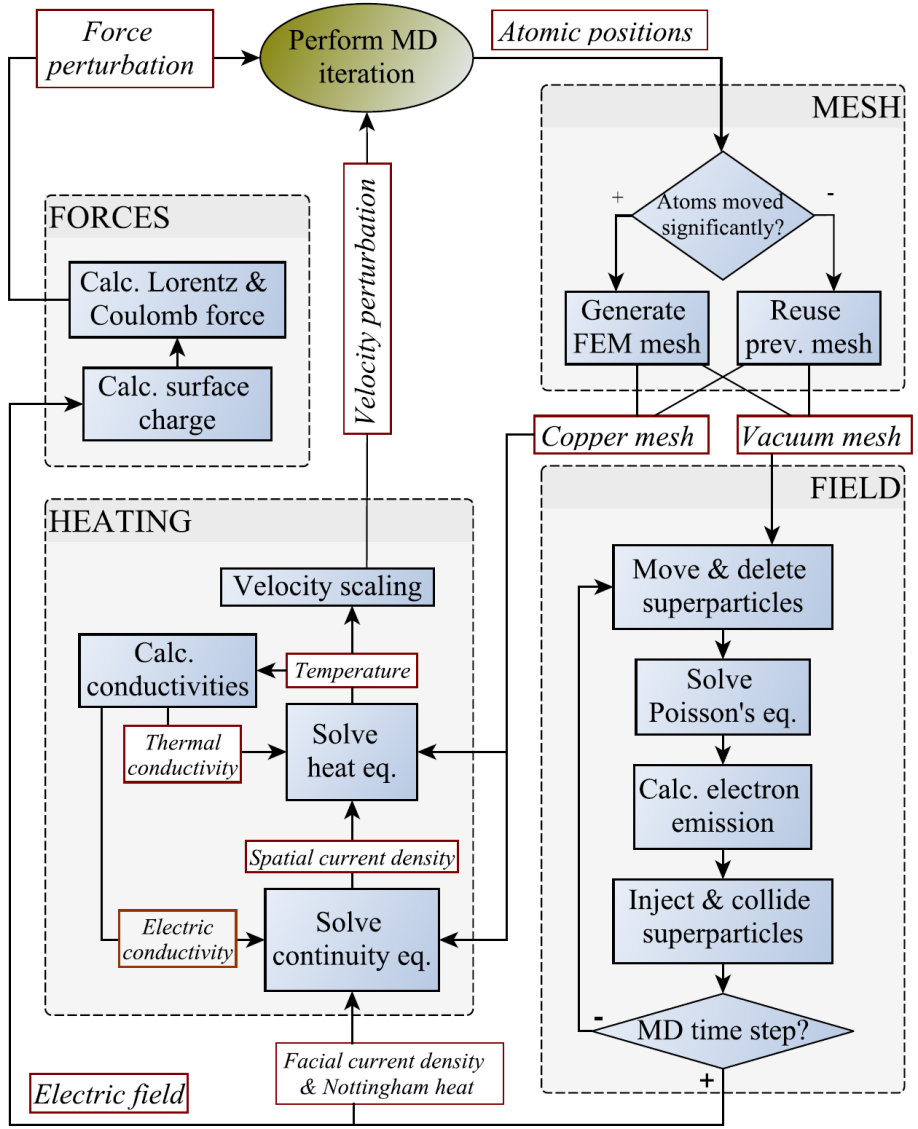
Molecular Dynamics:
- PARCAS MD
- LAMMPS

1. Mesh generation "on the fly" when MD system changes
2. Solve for **E**, T, **J** *et al.*
3. Feedback to MD electrostatic forces + heating

https://github.com/veskem/femocs

Specifics of FEMOCS algorithm

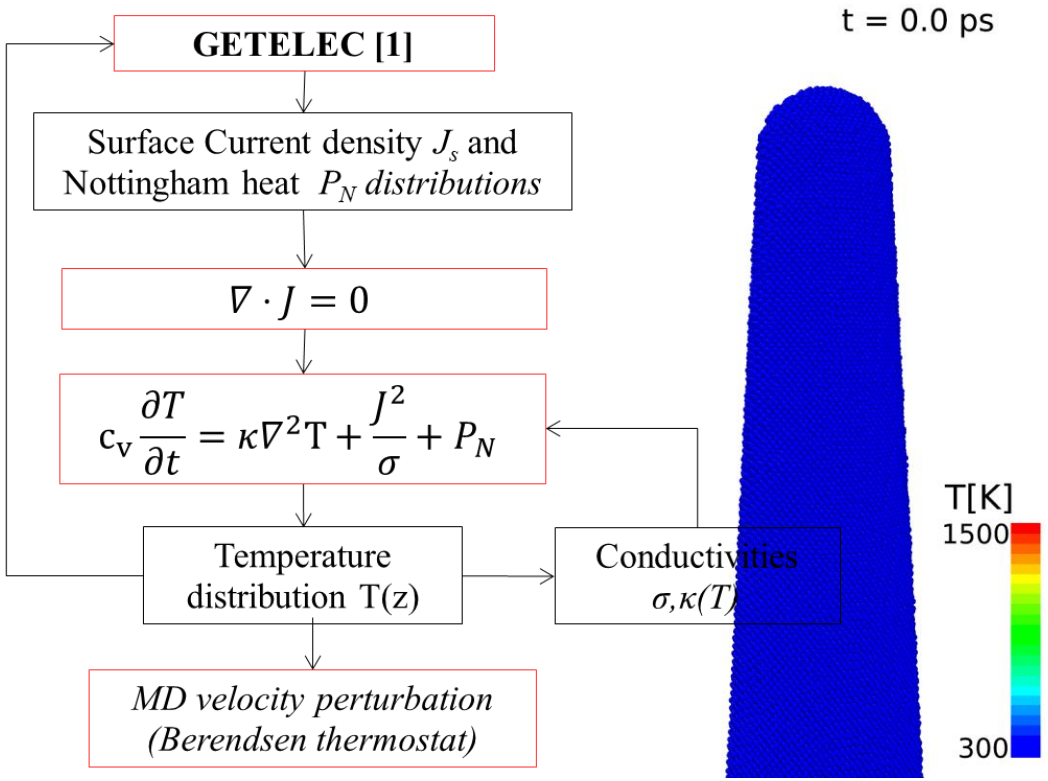




M. Veske et. al, Phys. Rev. E 101, 053307 (2020)

Heating and El. field calculations

Heating: Joule and Nottingham



The Electric field Calculation: Space Charge Screening effects

1. Track particles:

$$\vec{r}_i(t+\Delta t) = \vec{r}_i(t) + \vec{v}_i(t)\Delta t$$

$$\vec{v}_i(t+\Delta t) = \vec{v}_i(t) + \Delta t \frac{q_i}{m_i} \nabla \Phi$$

2. Interpolate charge density:

$$\rho(\vec{r}) = \sum_i w_i q_i U(\vec{r} - \vec{r}_i)$$

3. Collide particles (Monte Carlo method):

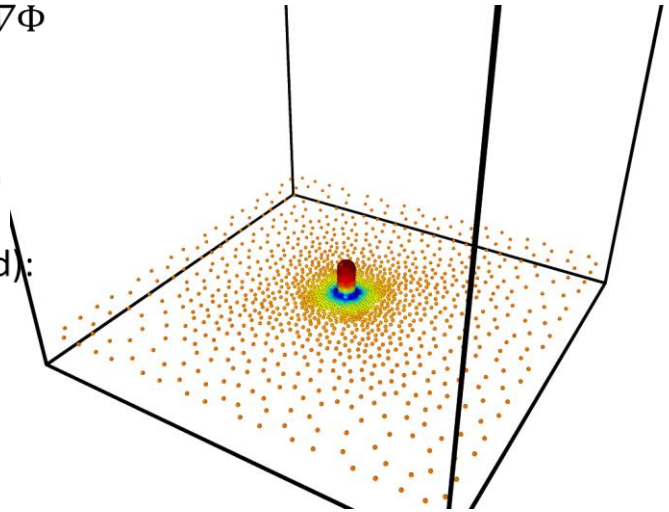
$$e^- + Cu \rightarrow Cu^+ + 2e^-$$

(… and many other collision types)

4. Solve Poisson equation (FEM)

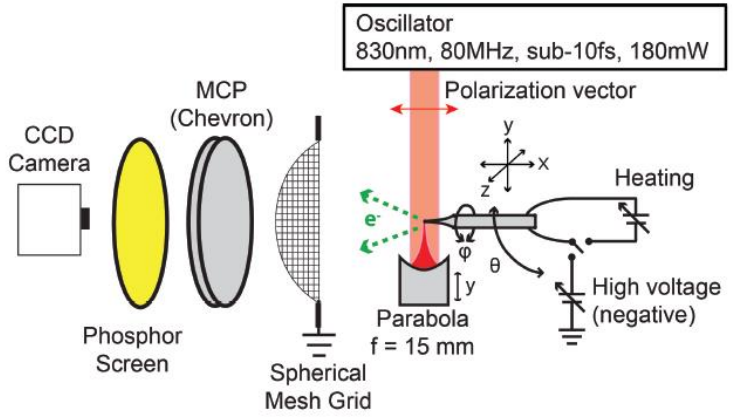
$$\nabla^2 \Phi = -\frac{\rho}{\epsilon_0}$$

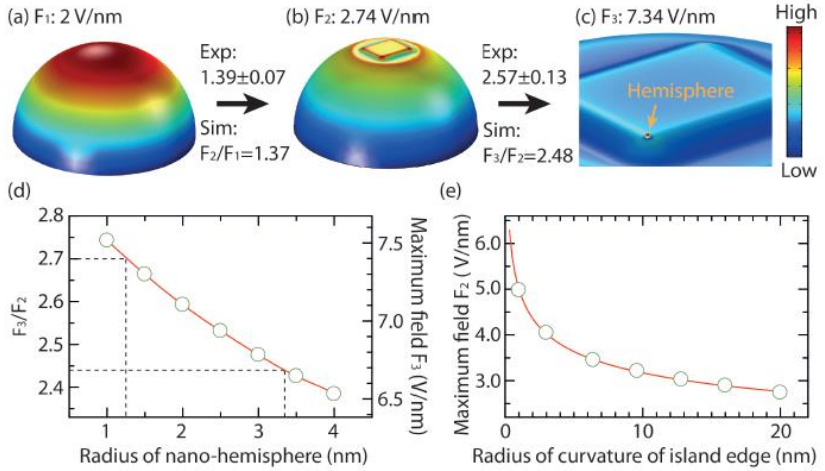
5. Calculate surface currents and inject new particles
6. Repeat for desired number of time steps



[1] A. Kyritsakis, F. Djurabekova, Comput. Mater. Sci 128 15

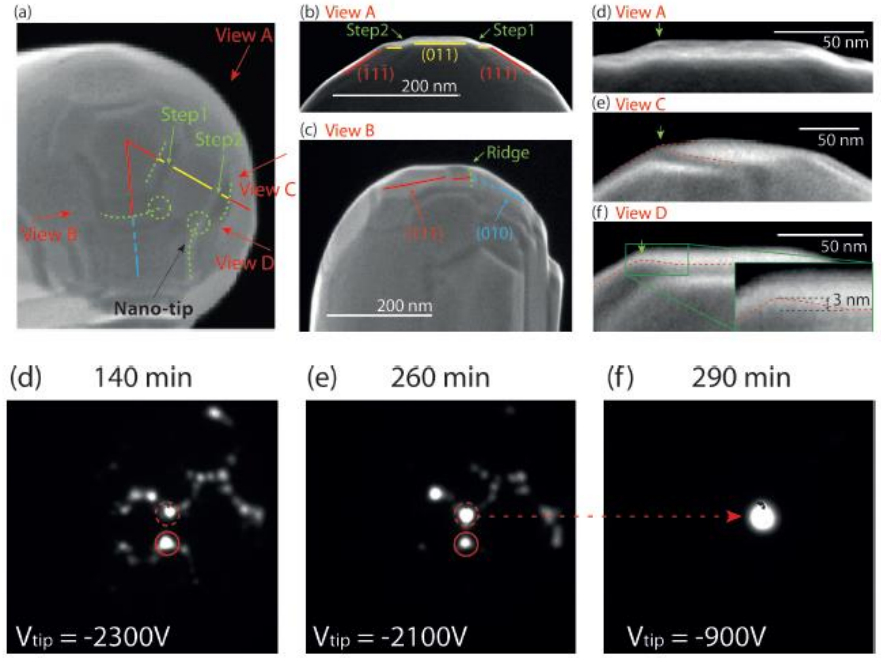
Static surface under el. field



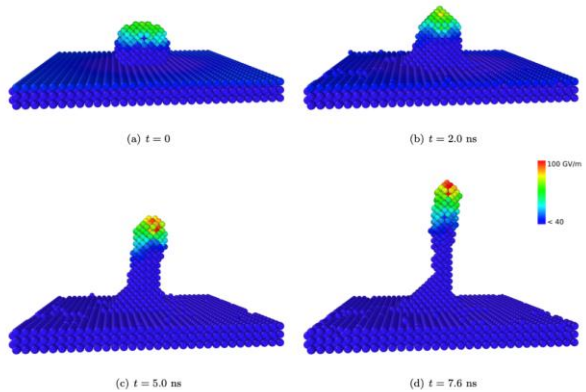


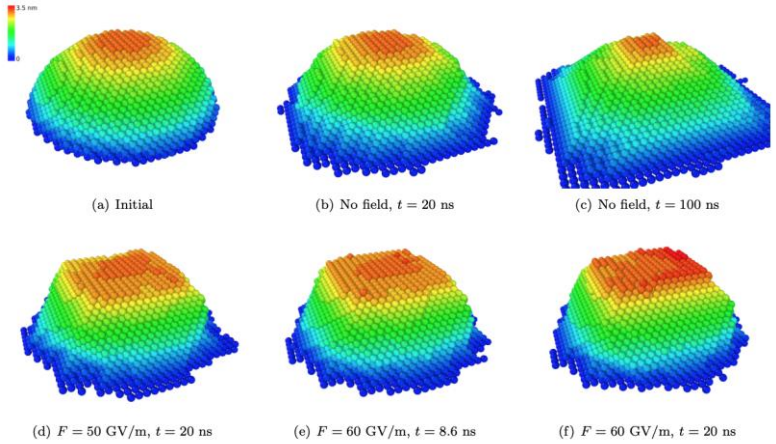
H. Yanagisawa, V. Zadin *et al.* https://arxiv.org/abs/1605.05393

- Field Emission Microscopy experiment
- Collaboration with Dr. Hirofumi Yanagisawa(Max-Planck Institute of Quantum Optics)
- Surface faceting and protrusion formation
- **Possible mechanism for emitter formation**



Current understanding





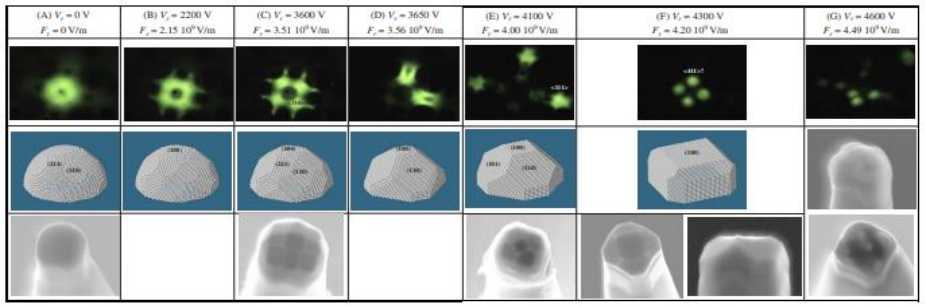
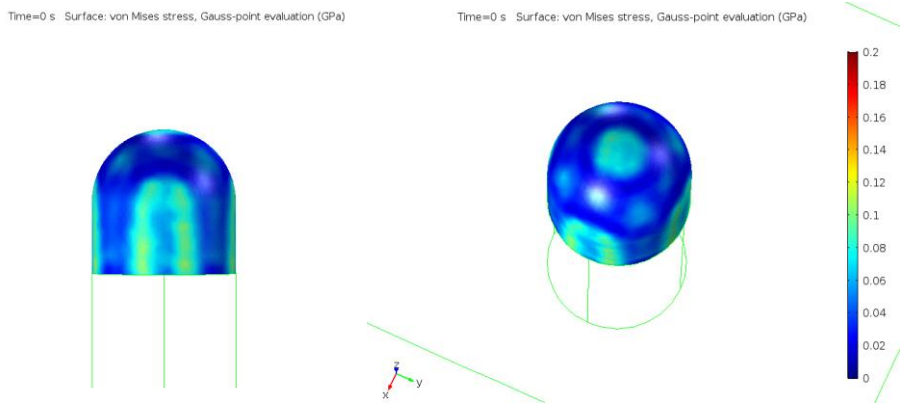
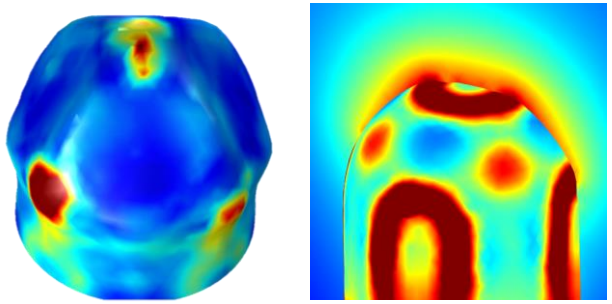
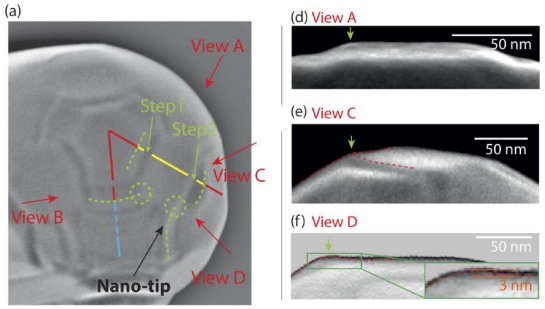


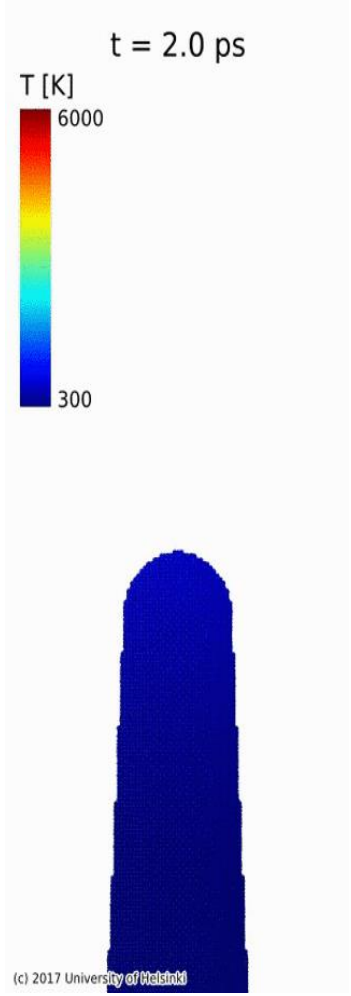
FIG. 5. (Color online) Summary of the evolution of the tip shape in the remolding process at the temperature T_r=2300 K. The FE patterns (second row), the emitter tip shape models (third row), and the SEM images of the tips at selected stages (fourth row) are given in the order of the increasing remolding voltage.

Fujita *et al.,* Phys. Rev. **75**, 2007



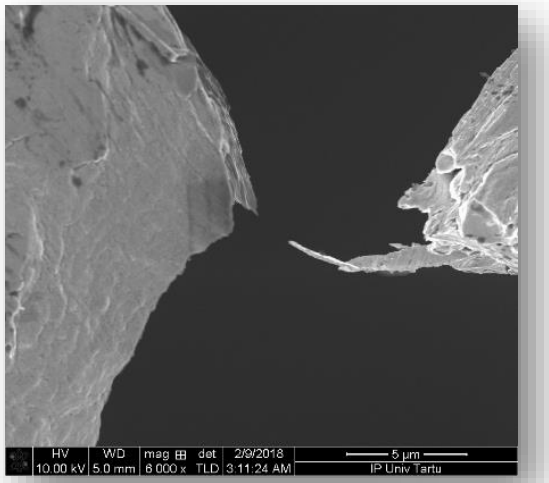


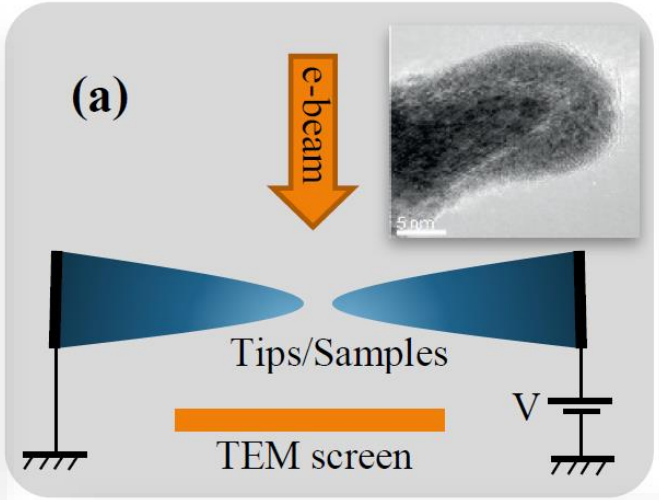


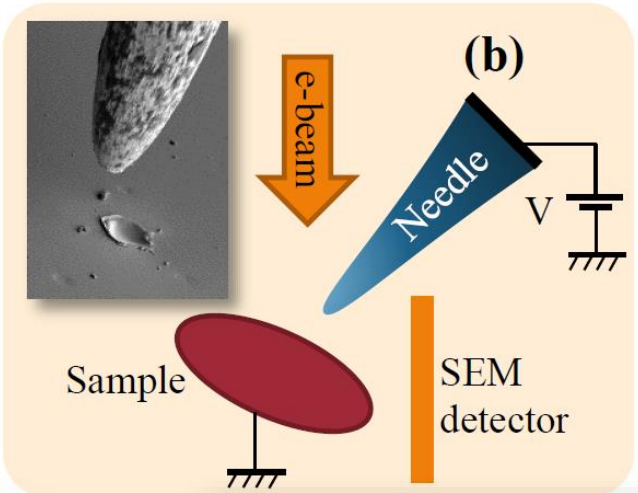


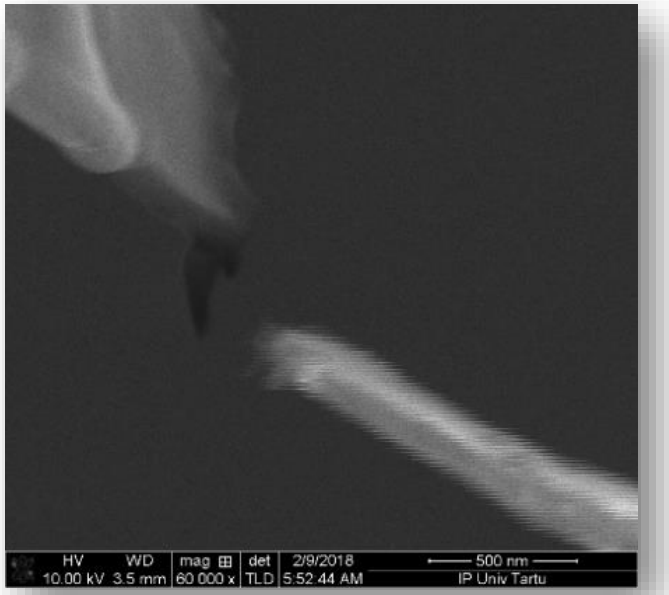
V. Zadin, University of Tartu

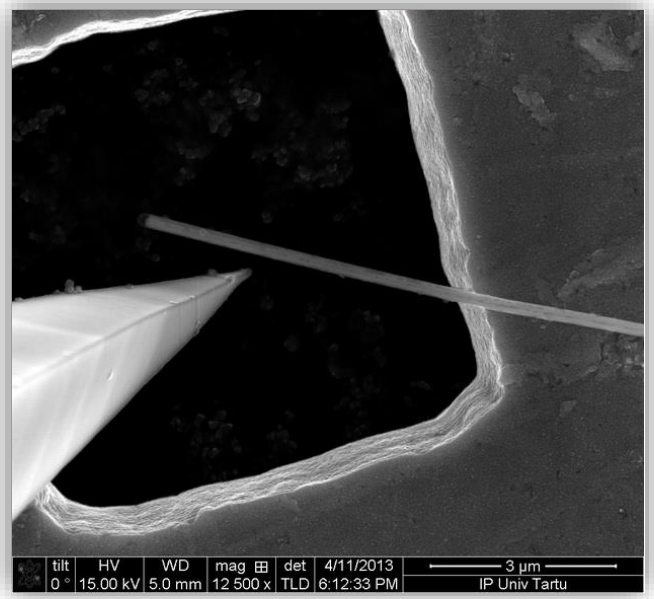
Field assisted surface diffusion: the experiment











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Conclusions

- FEMOCS – concentrates our best current understanding of BD onset
  - Still has significant limitations – emitter must be pre-created
- GETELEC – best currently available tool for field emission calculation & analysis
  - Nottingham heat
  - Metals & semiconductors
  - **Web interface to make it usable by wider audience**
- Whole multiscale range of simulations most probably needed to understand true reasons of BD initiation
- Tight integration with in-situ microscopy experiments critical!

Thank You for Your attention!

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