Multi-physics simulations of vacuum breakdown phenomena

Andreas Kyritsakis,

Institute of Technology, University of Tartu

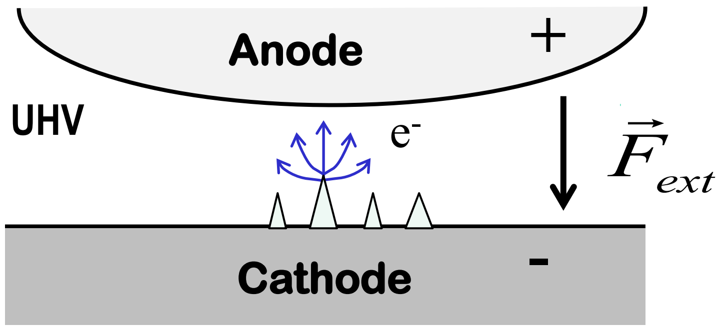
HG2021, 21.04.2021

Outline

- The 4 stages of vacuum breakdown development
- Stage 3:
  - Particle In Cell (PIC) Simulations
  - The missing initial vapor
- Stage 2:
  - Concurrent ED-MD simulations on nanotips
  - The thermal runaway process
  - Integration with PIC
  - Space Charge effects in field emission
- Stage 1:
  - Atom diffusion on metal surfaces under high electric field

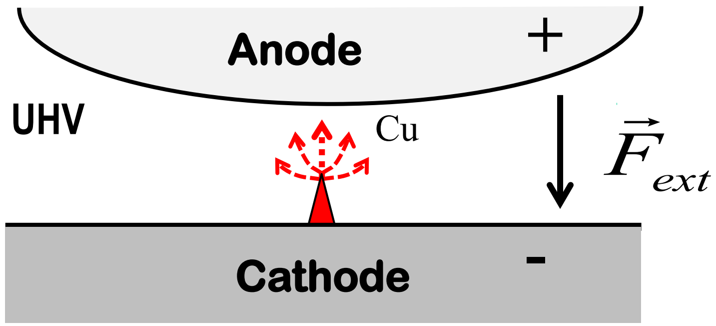
Vacuum breakdown stages

Stage 1 (μs-s)



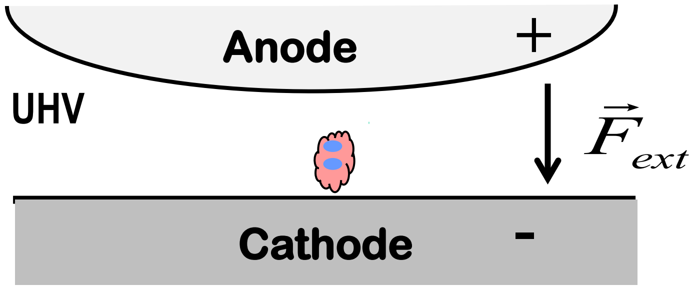
Formation of emission spots on surface, field enhancement

Stage 2 (~ns)



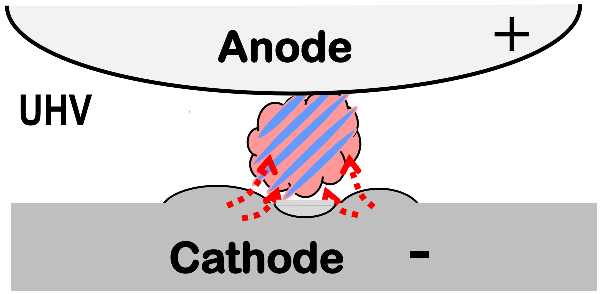
Tip thermal runaway, neutral evaporation

Stage 3 (~ns)



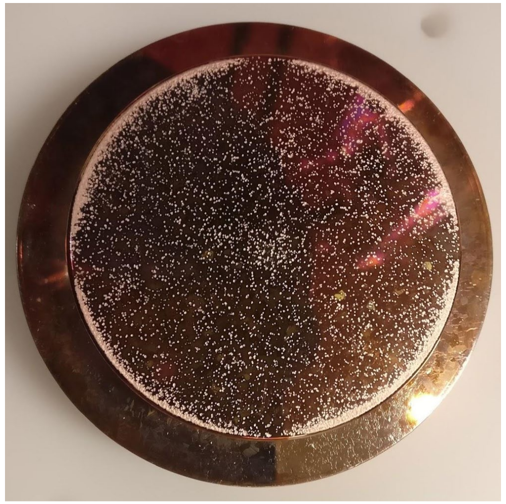
Ionization runaway, plasma formation, high current, voltage collapse

Stage 4 (10ns-μs)

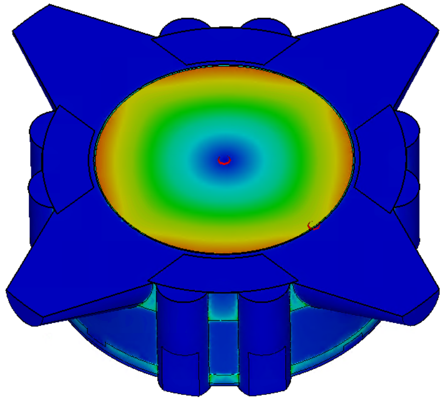


Plasma expansion, current rise, voltage collapse, surface damage

Importance of stages 2,3: power limits



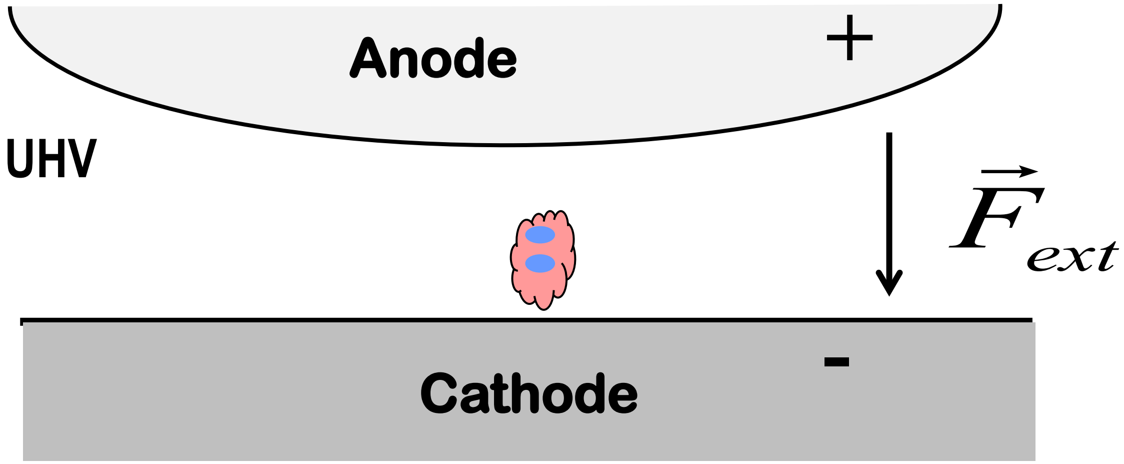
Soft Cu electrode,
Anton Saressalo



Calculated S_c @ 100 MHz
Jan Paszkiewicz

- Can we use this as a design way to mitigate Vacuum breakdown?
- First, we need to understand it
- What is the limiting factor for BD initiation?
- What makes the available EM power to be sufficient in some cases, while insufficient in other?

Stage 3 (~ns)



Ionization runaway, plasma formation, high current, voltage collapse

Particle In Cell method

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):

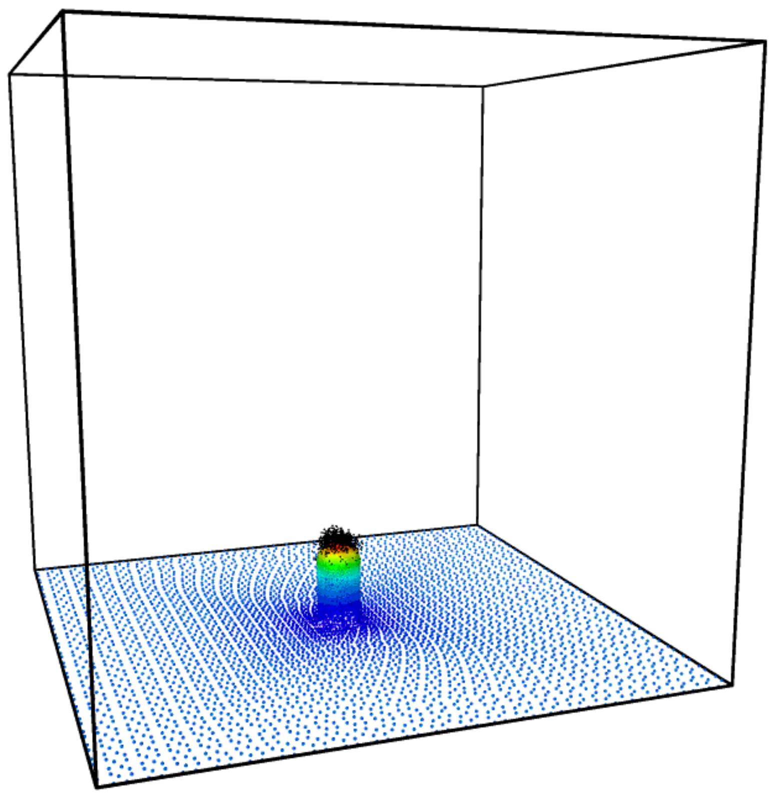
$$e^- + Cu \rightarrow Cu^+ + 2e^-$$

(… and many other collision types)

4. Solve **Poisson** equation (FEM)

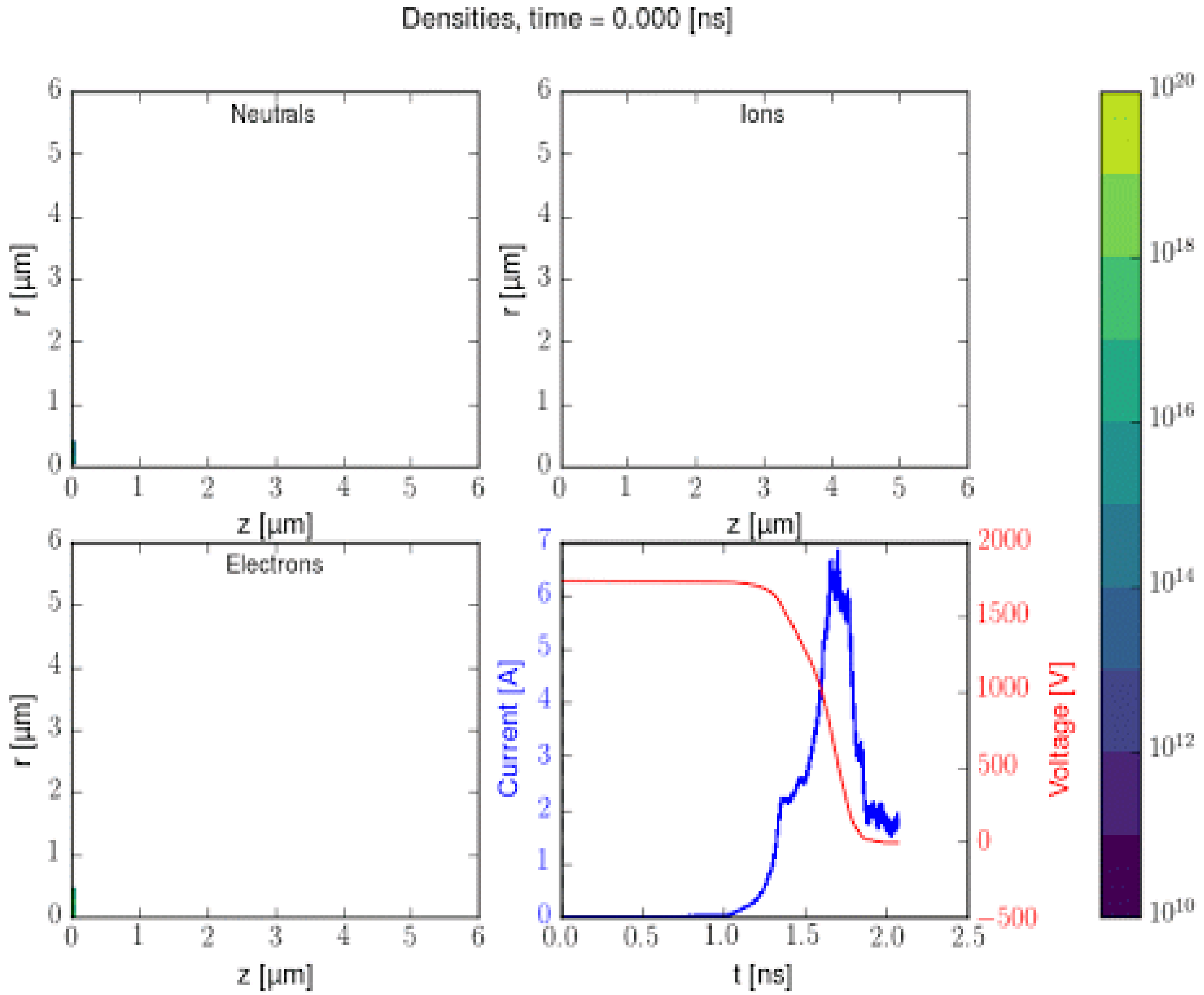
$$\nabla^2\Phi = -\frac{\rho}{\epsilon_0}$$

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



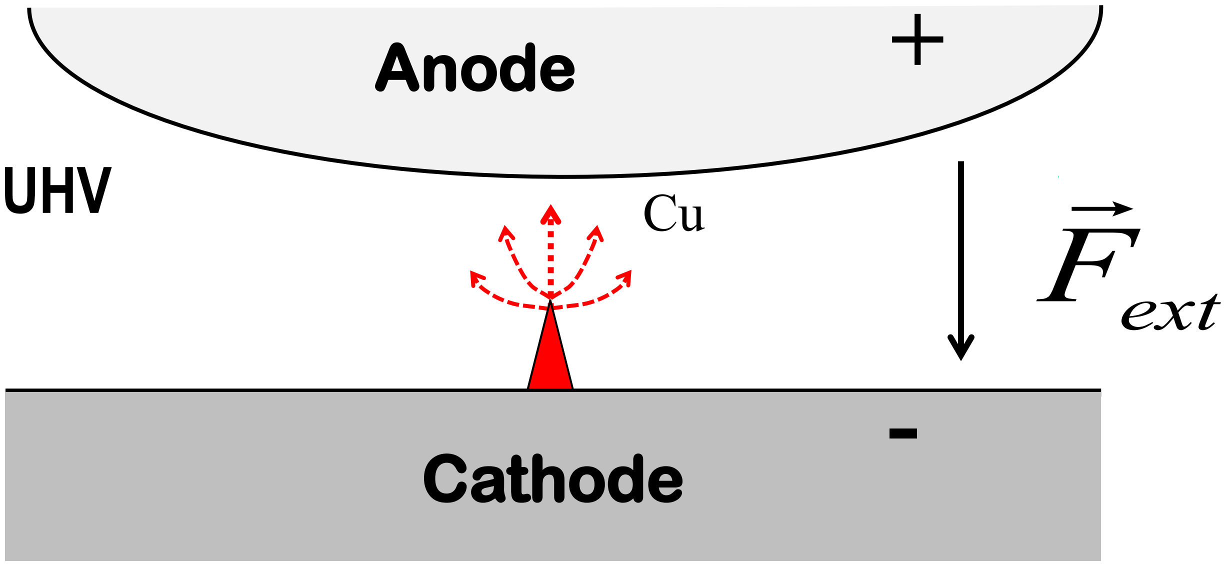
ArcPIC

- Plasma can ignite emitter assuming a small tip that:
  - Emits e with an enhancement β>35
  - Evaporates 0.015 Cu/e.
- What are the mechanisms in **Stage 2** that produce the necessary vapor?



H. Timko et. al., Contrib. Plasma. Phys. 4, 229 (2015). Animation by K. Sjobaek

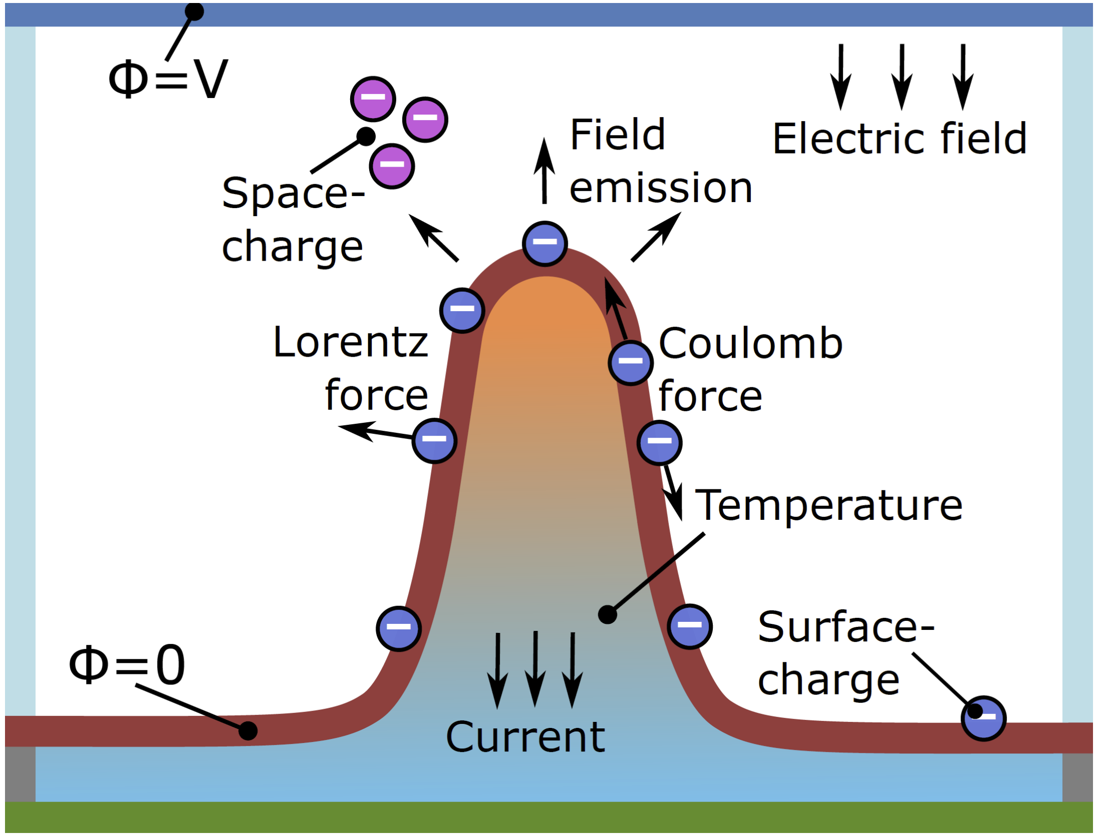
Stage 2 (~ns)



Tip thermal runaway, neutral evaporation

Multi-physics simulations

- Thermal runaway: **complex** process that involves various phenomena in various space scales
- Need for **concurrent, multi-scale, multi-physics** simulations

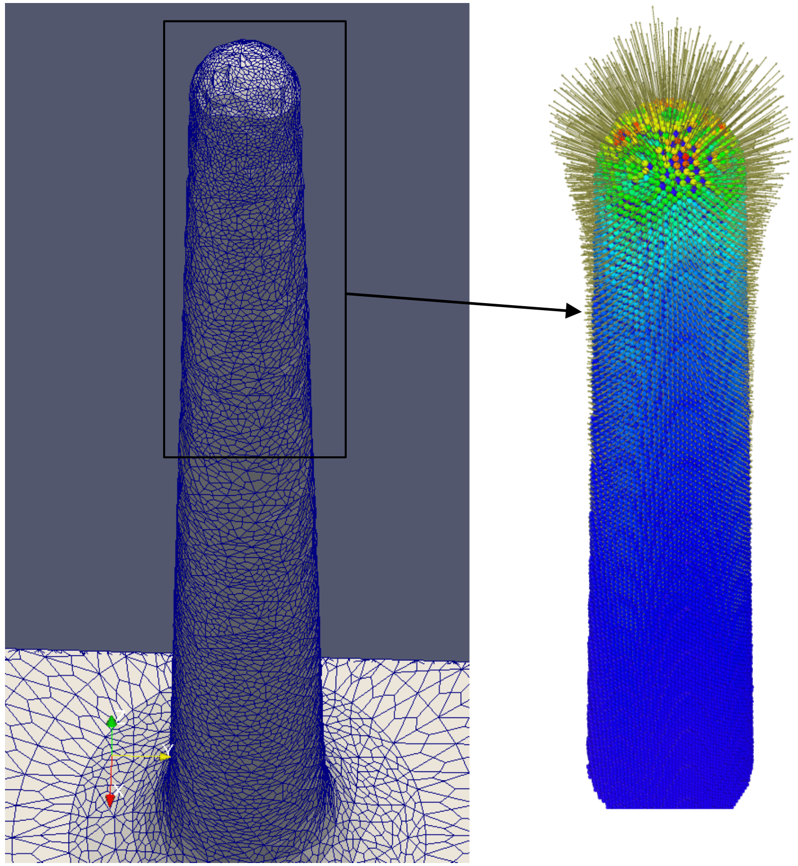


Concurrent MD-FEM

1. Mesh generation “on the fly” when MD system changes
2. Solve the Poisson equation

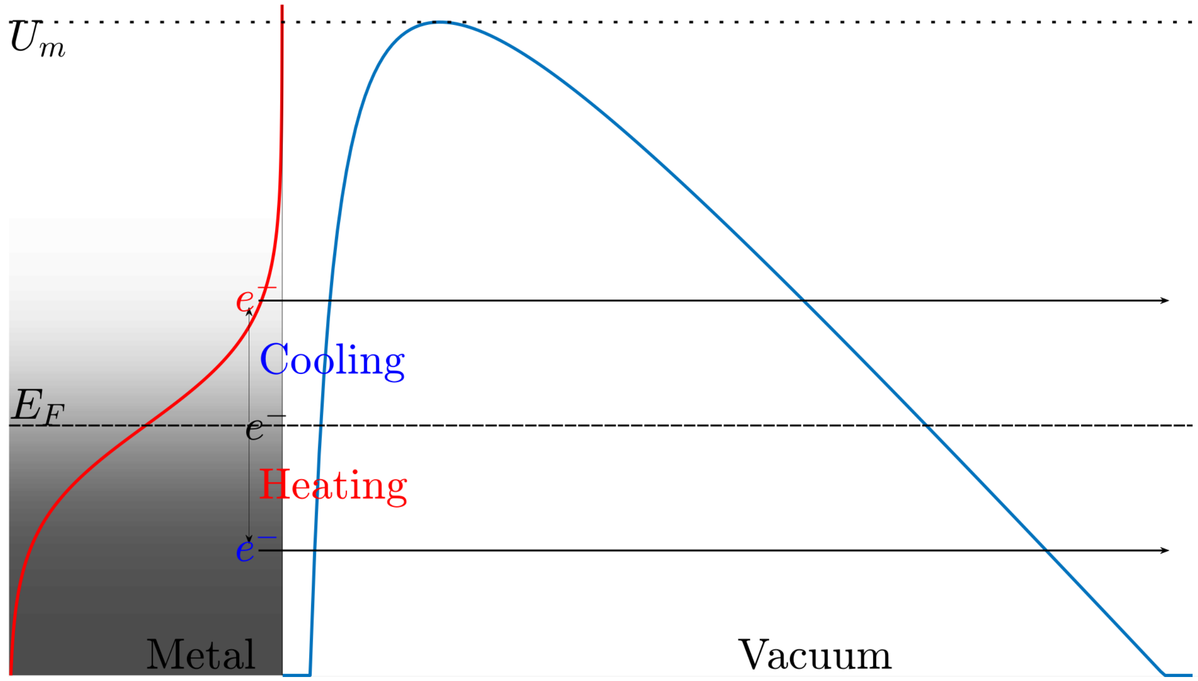
$$\nabla^2 \Phi = -\frac{\rho}{\epsilon_0}$$

3. Feedback to MD electrostatic forces + heating

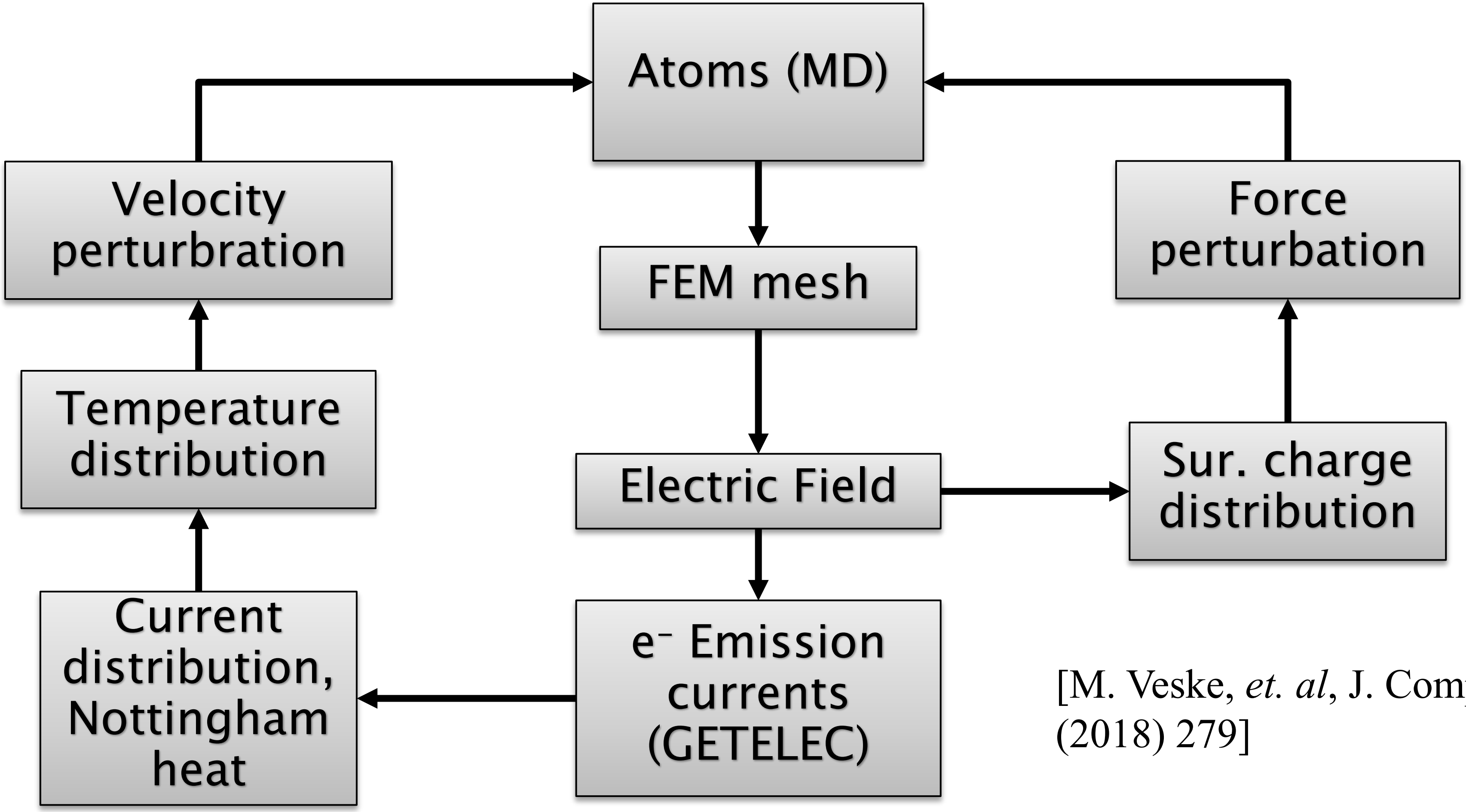


Thermal effects of electron emission

- Two heat deposition components:
  - ✓ Joule heating $P_J = J^2/\sigma$
  - ✓ Nottingham heat (surface heat deposition)
    $P_N(F,T)$
    $= \int (E(\vec{k}) - E_F) f_{FD}(\vec{k};T) D(\vec{k}) d^3k$
    $= J_s \langle E - E_F \rangle / e$

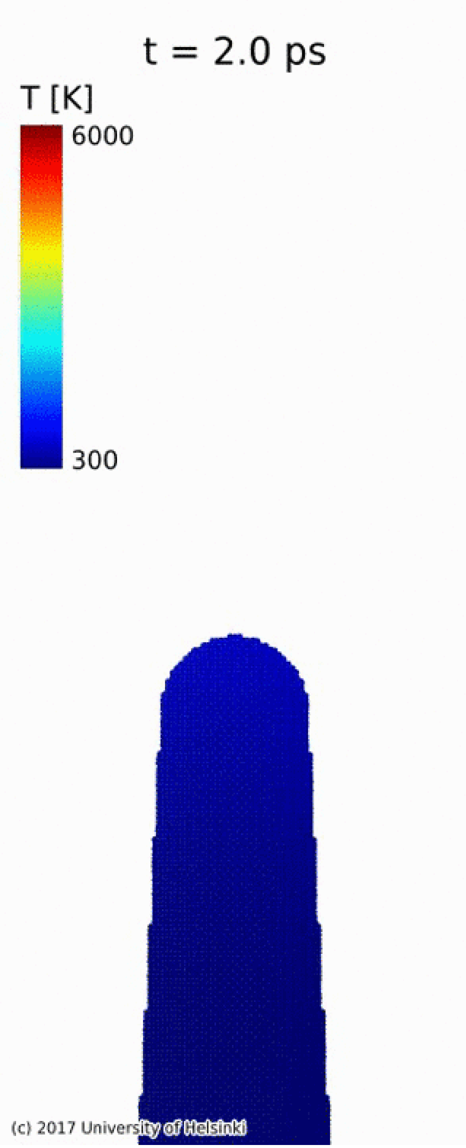


The concurrent algorithm (FEMOCS)

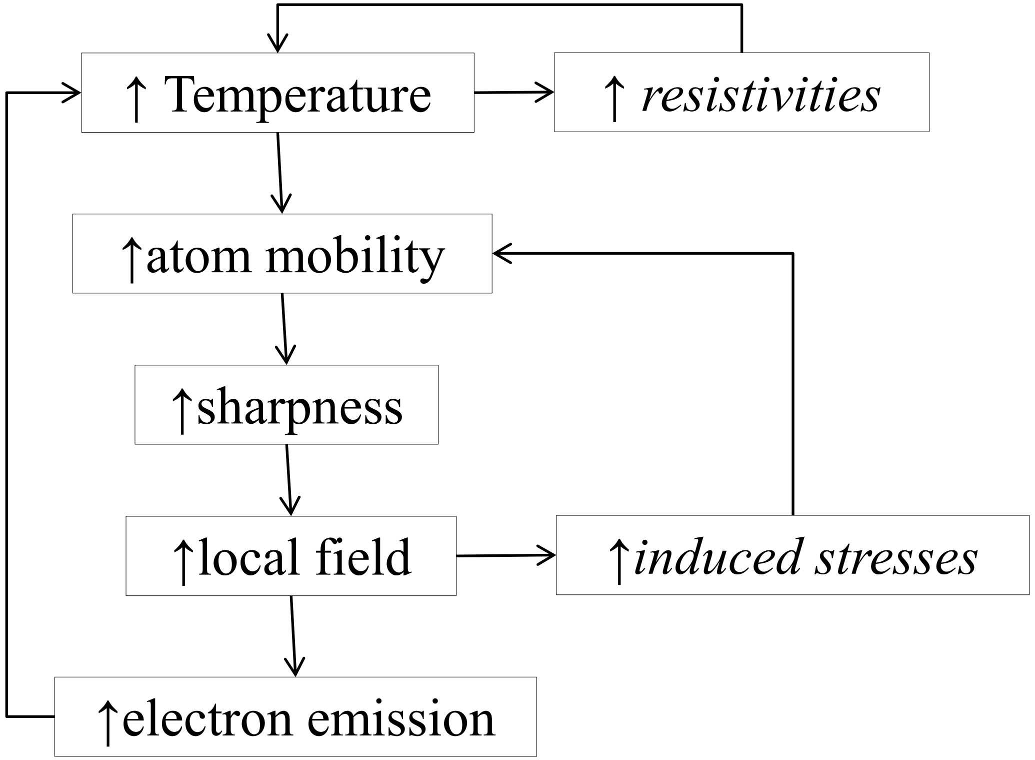


[M. Veske, *et. al*, J. Comp. Phys. 367 (2018) 279]

Thermal runaway



Thermal runaway:



Evaporation of large parts of the tip in forms of atoms and nanoclusters

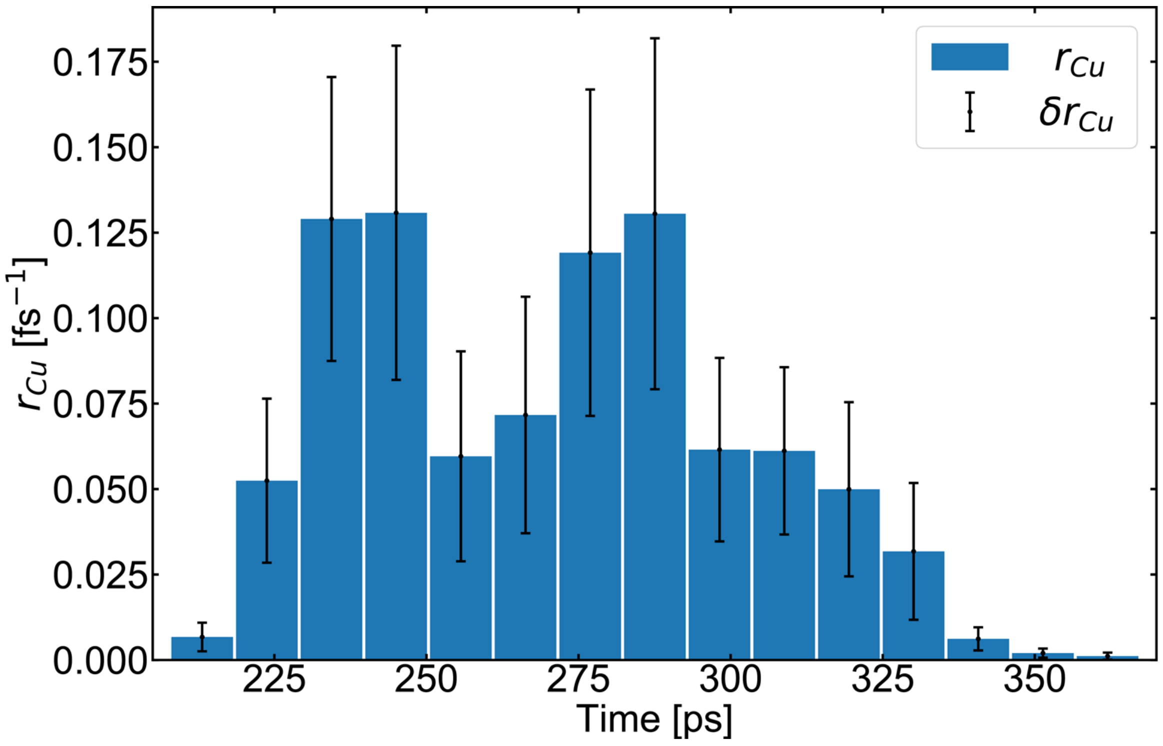
[A. Kyritsakis et. al., *J. Phys. D: Appl. Phys.* **51** 225203 (2018)]

Evaporation events

- Mean evaporation

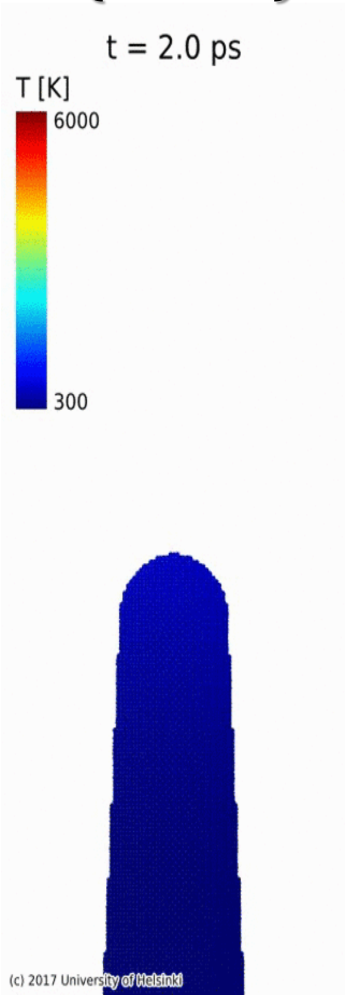
  R_{Cu}= 75±11 atoms/ps
- Mean current I = 2807±153 e/ps
- $R_{Cu/e}$= 0.025±0.003 atoms/e
- **Exceeds** the minimum 0.015 found

  by plasma simulations

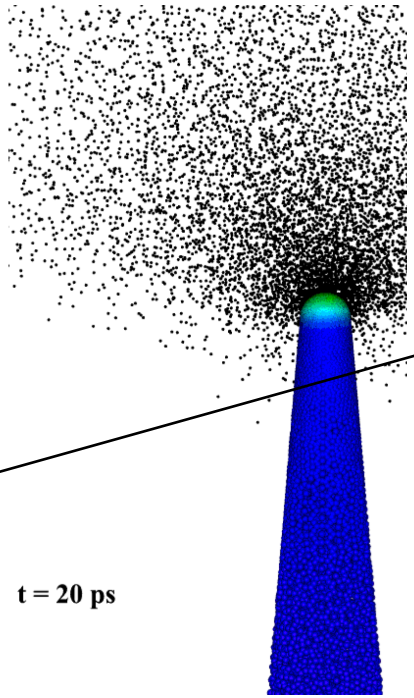


Connecting stages 2 and 3

Stage 2 (MD-ED)

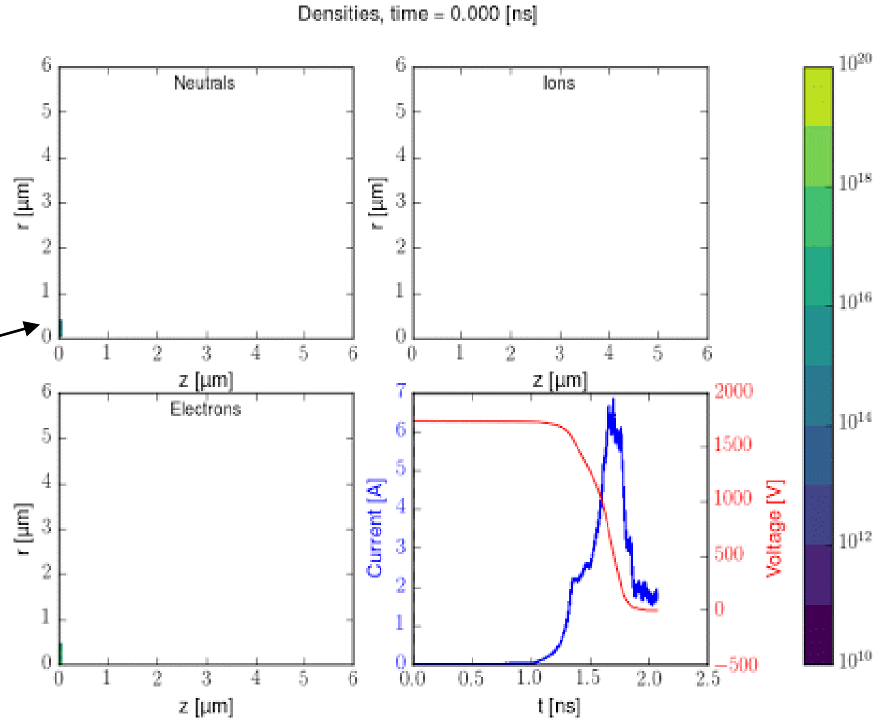


Stage 2&3 (MD-FEMOCS-PIC)

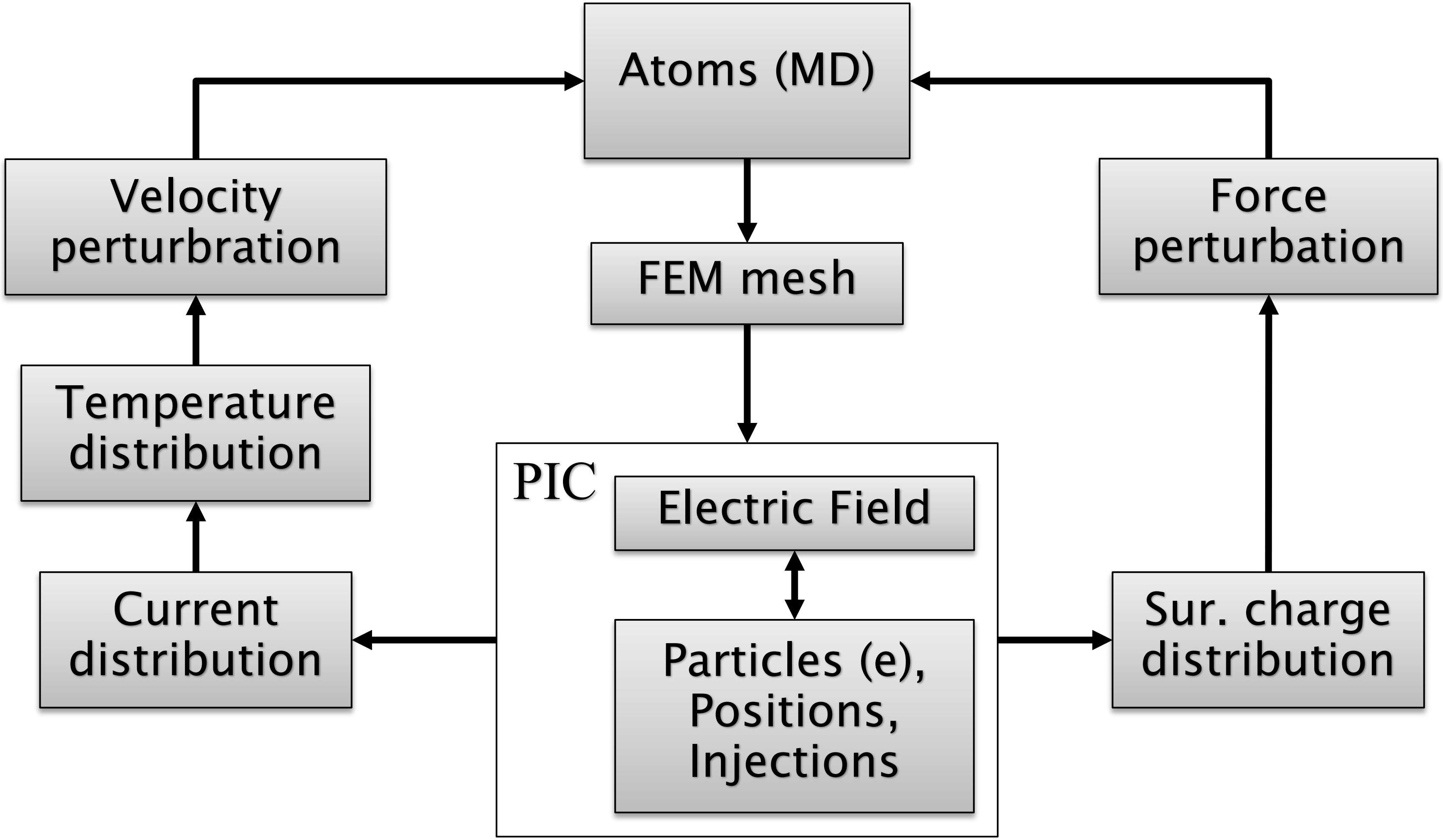


t = 20 ps

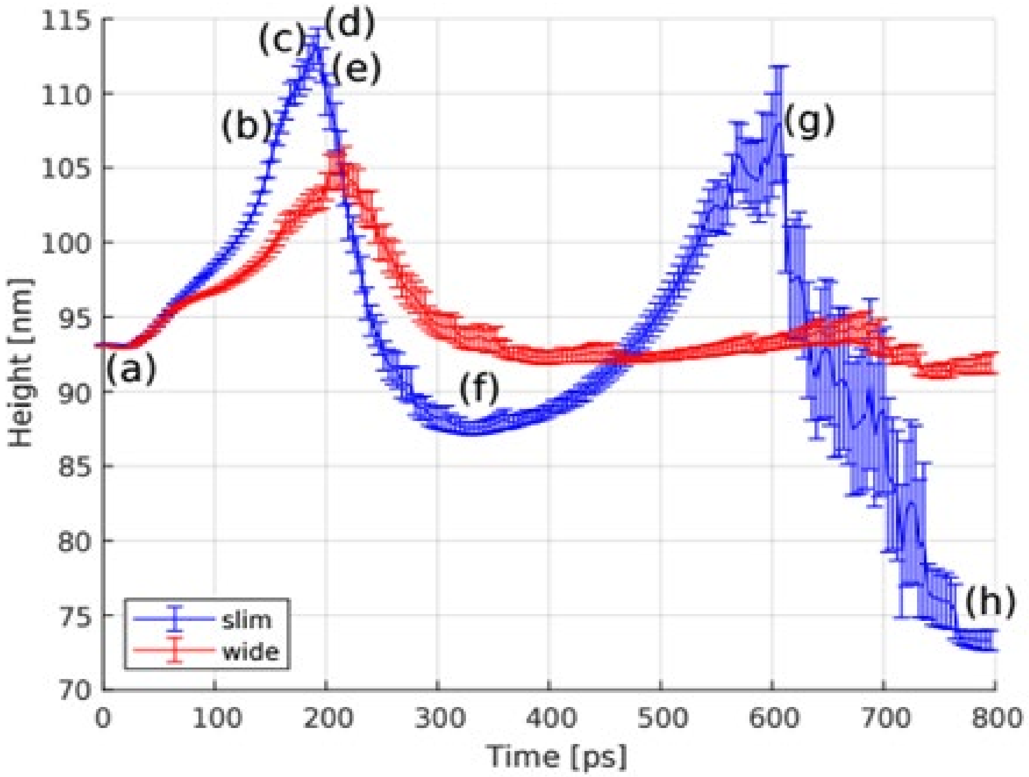
Stage 3 (PIC)



Incorporating PIC in FEMOCS



Results including PIC (SC effects)



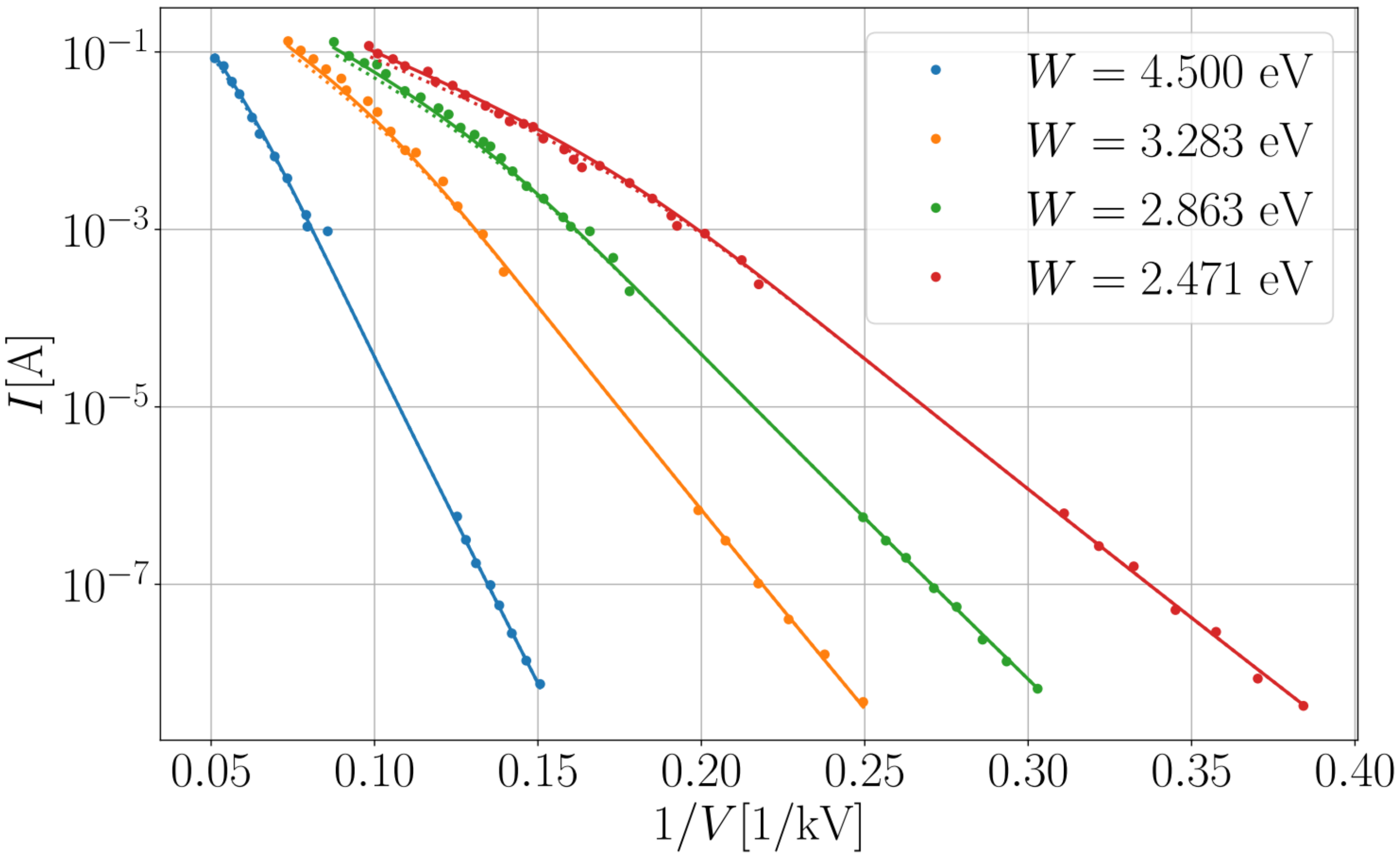
M. Veske et. al, Phys. Rev. E 101, 053307 (2020)

General Space Charge Scaling

Comparison against experiment (Barbour *et al*, Phys. Rev. 92, 45 (1953))

Geometry–dependent correction factor

$$F = F_L - \frac{4}{3}\omega\frac{kJ_s\sqrt{V}}{F_L}$$



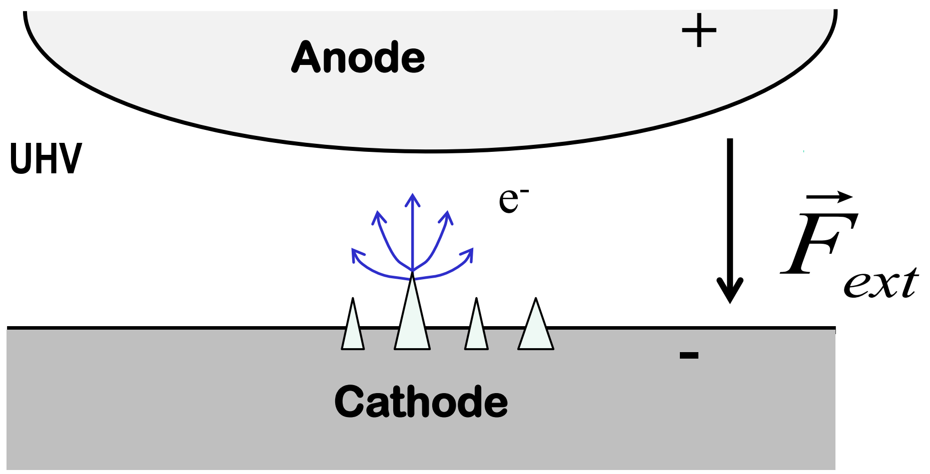
[A. Kyritsakis et. al. arXiv:2008.11984
(under review in New. J. Phys.]

Outlook & on-going work

- Final goal:
  - Simulation of the full BD process
  - Understanding the limitations of:
    - ✓ Power flow (R_{BD})
    - ✓ Tip size, shape, β, etc

- On-going development:
  - ✓ More plasma species (Cu, Cu^{+}, Cu^{++} …)
  - ✓ Bombardment heating
  - ✓ Direct field ionization
  - ✓ Coupling to external circuit - $Z_{BD}(\omega)$
  - ? Fully coupled MD-PIC:
    - ? Boundary injection
    - ? Two temperature model

Stage 1: Emitter growth



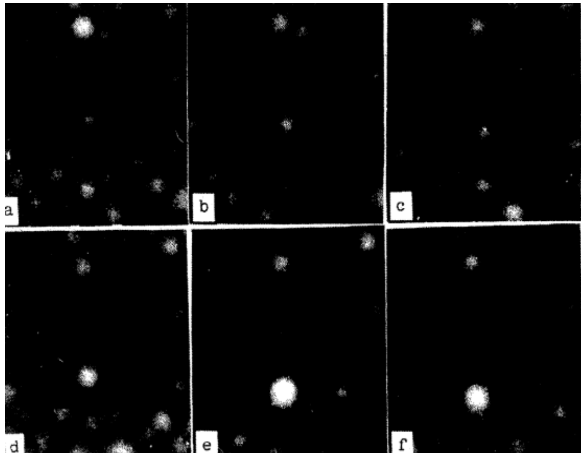
Formation of emission spots on surface, field enhancement

- Existing hypotheses:
  - Deposition of adsorbents
  - Surface diffusion under field
  - Dislocation movement
  - macroparticles

Fundamental question

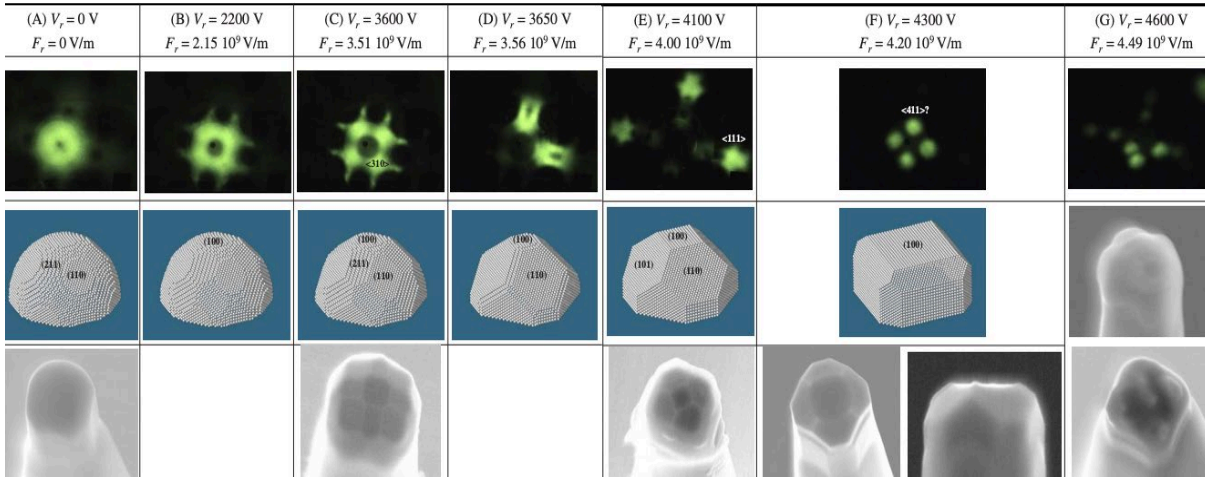
- ➢ How are migration barriers affected by high electric fields ?
- ➢ Experimental evidence of field effects are known experimentally since the 60s

❑ Directional diffusion of W adatom on W {110} surface



[1] T. T. Tsong and G. L. Kellogg, Phys. Rev. B 12, 1343 (1975).

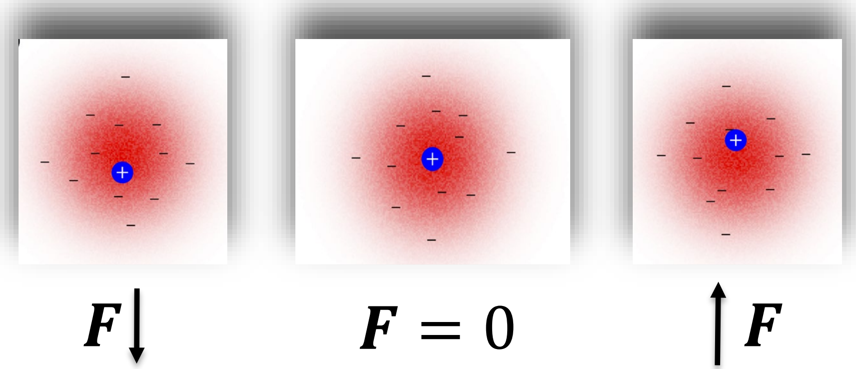
❑ W tips diffusing into different shapes when flashed under high field



[2] S. Fujita and H. Shimoyama, Phys. Rev. B 75(23), 235431 (2007).

Free molecules under high field

- Isolated atom under field F
  - Total dipole moment: $p(E) \approx \mu + \alpha F$
  - Energy under field: $U(E) = U_0 - \int_0^F p dF = U_0 - \mu F - \frac{1}{2}\alpha F^2$
  - The atom is attracted towards higher F

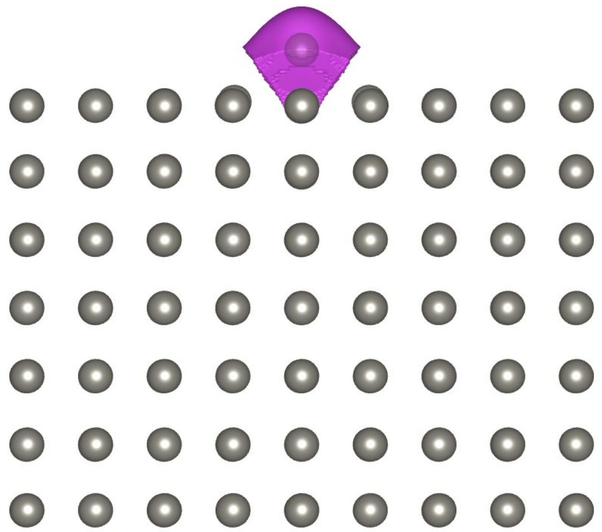


Adatoms under high field

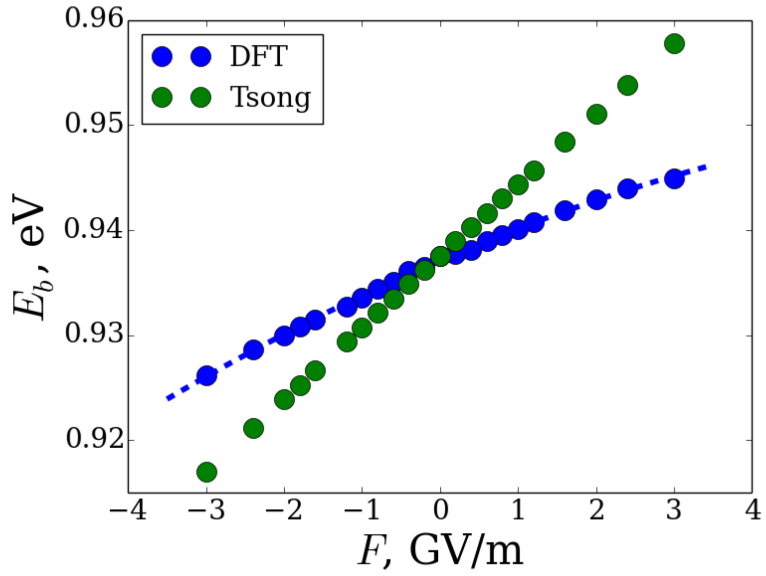
- First trial: like free atoms, but with variable μ,α (Tsong & Kellogg 1975)

$$E_m = E_0 - \mu_s F_s + \mu_l F_l - \frac{1}{2}\alpha_s F_s^2 + \frac{1}{2}\alpha_l F_l^2$$

- But how is the atomic dipole defined?
- Let's define it from atomic partial charges



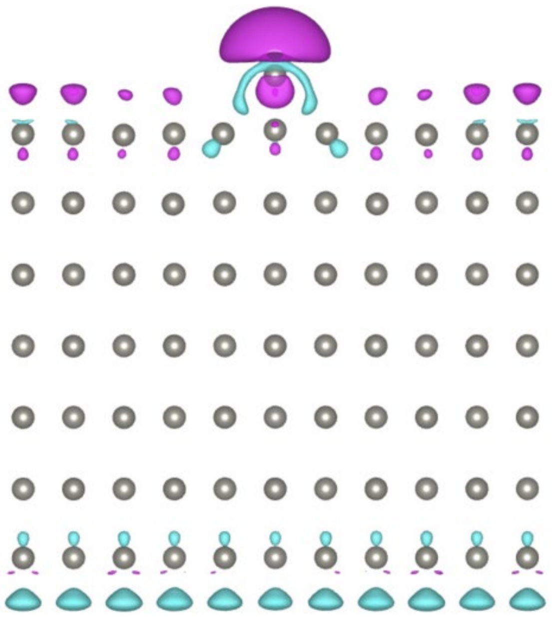
- BUT: no agreement with DFT



Considering the atomic environment

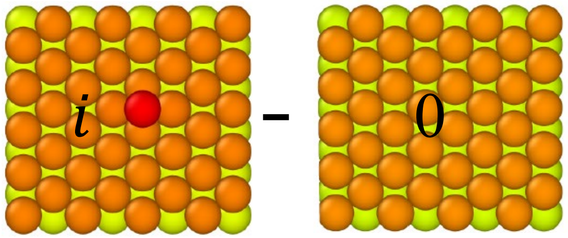
$$P = \int_V \rho \vec{r} d^3 r = \mathcal{M} + AF$$

$$E = E_0 - \mathcal{M}F - \frac{1}{2}AF^2$$



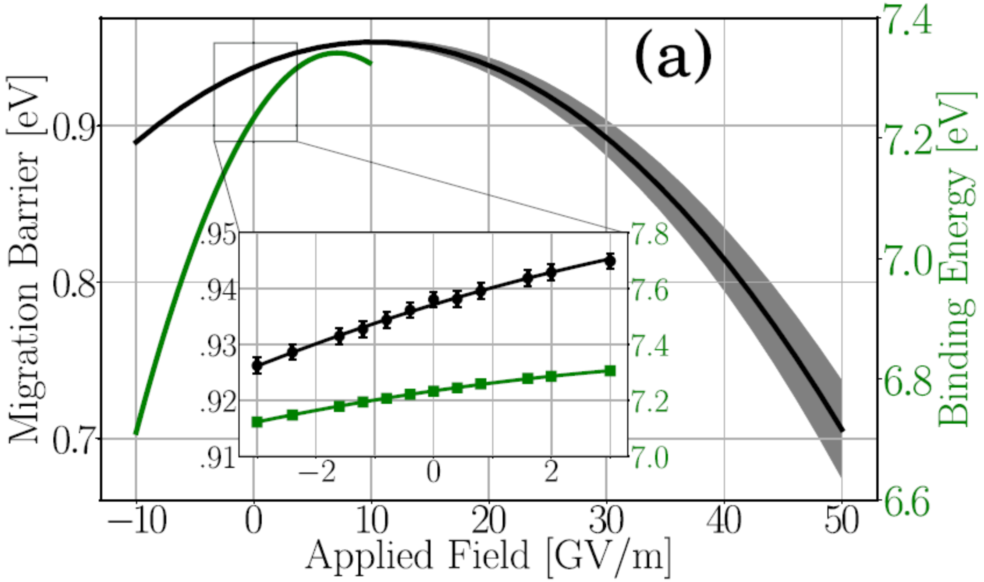
[1] A. Kyritsakis, E. Baibuz et. al., Phys. Rev. B 99 (2019) 205418

Define $p_i = P_i - P_0$ ($\alpha_i = A_i - A_0, \mu_i = \mathcal{M}_i - \mathcal{M}_0$)



- Barrier (no F gradient)

$$E_m(F) = E_m(0) - (\mu_s - \mu_l)F - \frac{1}{2}(\alpha_s - \alpha_l)F^2$$



Biased diffusion

$$E_m(F) = E_m(0) - (\mu_s - \mu_l)F - \frac{1}{2}(\alpha_s - \alpha_l)F^2$$
$$-\Delta F(\mu_s + \alpha_s F_l)$$

Bias coefficient:

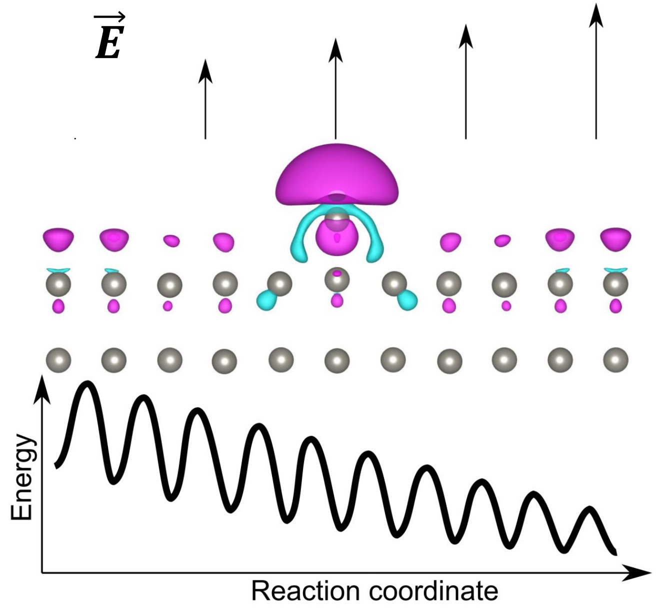
- extracted from experimental drift velocity:

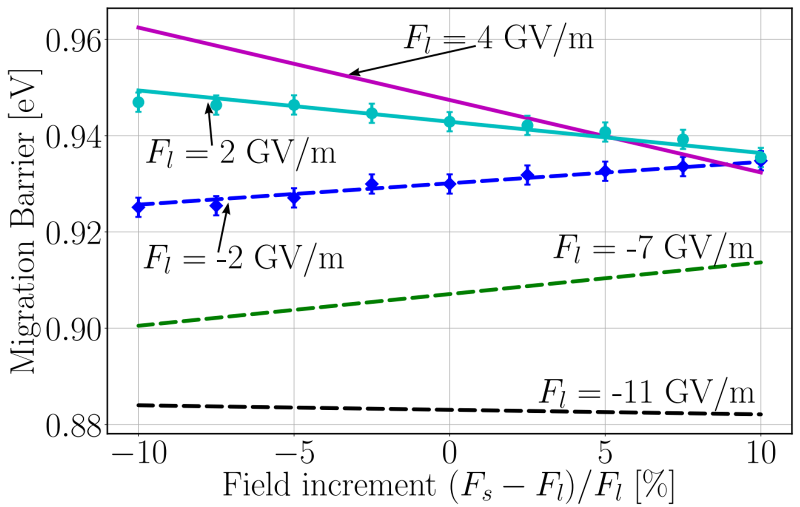
  $B = 1.14 \pm 0.25 e\text{Å}$

- Our calculations:

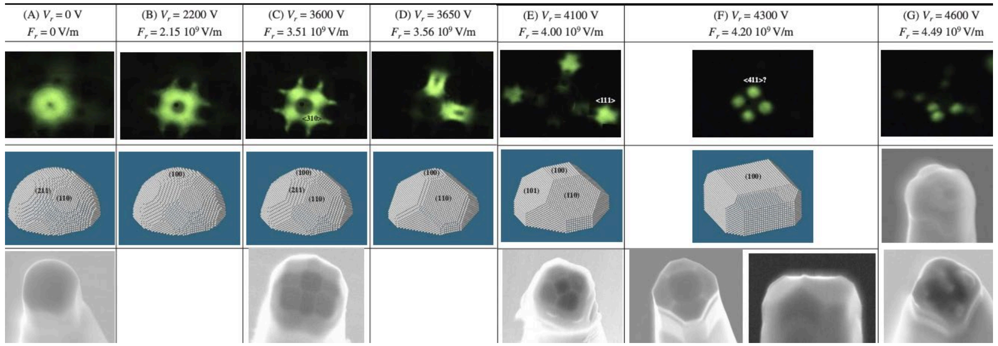
  $B = 0.88 \pm 0.03 e\text{Å}$

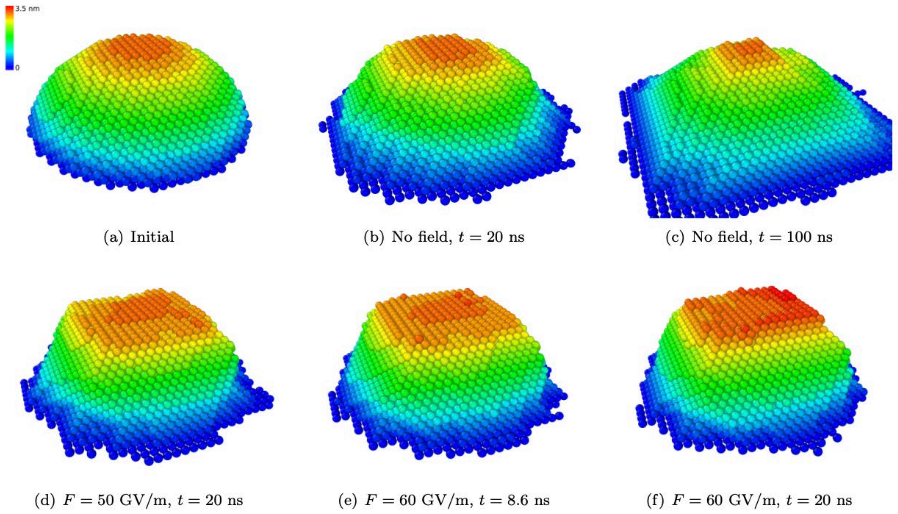
- Good agreement!



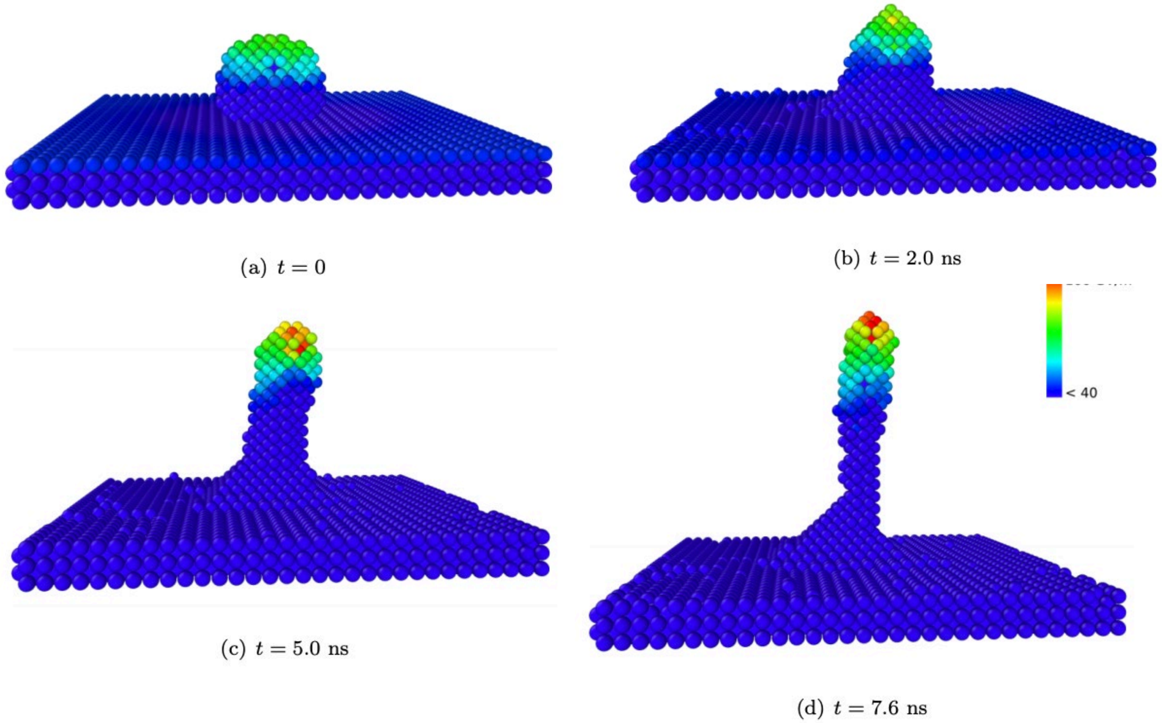


Tip growth in high electric field





V. Jansson, et. al., Nanotechnology 31, 355301 (2020)



- Tips can grow under high field
- BUT:
  - we had to exaggerate F and T
  - All μ,α are taken equal to W on W{110}

Conclusions

- Stages 2 & 3:
  - Multi-physics simulations are necessary to understand the VBD development
  - Thermal runaway of metal tips releases vapor necessary to start plasma
  - Further development of hybrid MD-PIC necessary to understand plasma formation and dependence on power

- Stage 1:
  - Preliminary results on surface diffusion under high electric field indicate that tips can grow
  - Further calculations are required to consider different polarization characteristics

Thanks to all contributing co-workers

- University of Tartu:
  - Vahur Zadin
  - Mihkel Veske
  - Kristjan Eimre
  - Ihar Suvorau
  - Sergei Vlassov
  - Sven Oras
- University of Helsinki:
  - Flyura Djurabekova
  - Ville Jansson
  - Ekaterina Baibuz
  - Roni Koitermaa
- CERN:
  - Kyrre Sjobaek
  - Walter Wuensch
  - Sergio Calatroni

THANK YOU