
AND NOW FOR
SOMETHING
COMPLETELY
DIFFERENT

Atomistic simulations of field evaporation in atom probe tomography

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What is APT?

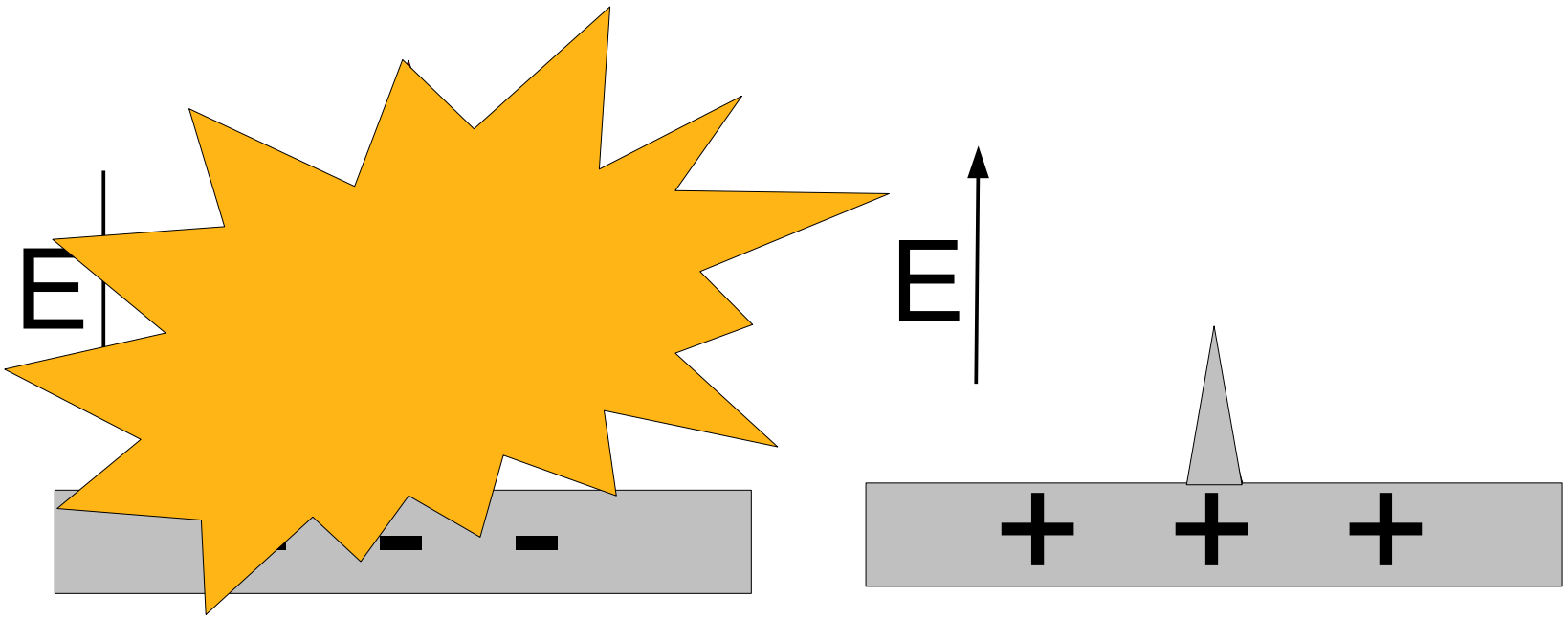
- Method to determine the structure and chemical composition of a sample in 3D
- Very high resolution (~nm)
    - Atomic resolution is the ultimate goal
- Destructive method

(Cameca SAS)

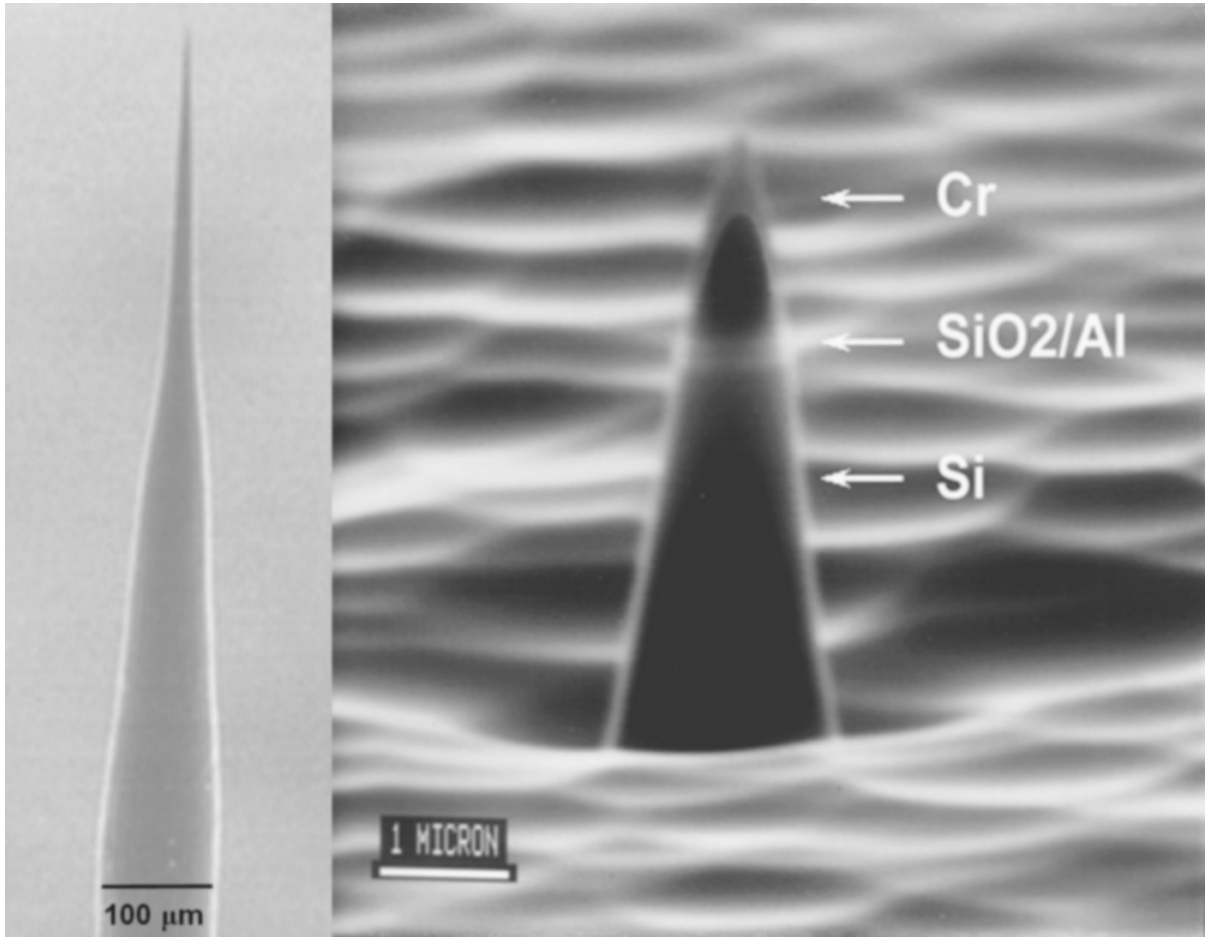
Why should you care?

- Our work is an offshoot from breakdown related research
  - Branching out is good!
  - Increased cooperation between communities
- Somewhat relevant for RF case (not so much DC)
  - What happens at the anode
- Field evaporation may increase field needed for breakdown to occur

To break down or not?



How it works



(Kelly et al. 2007)

How it works

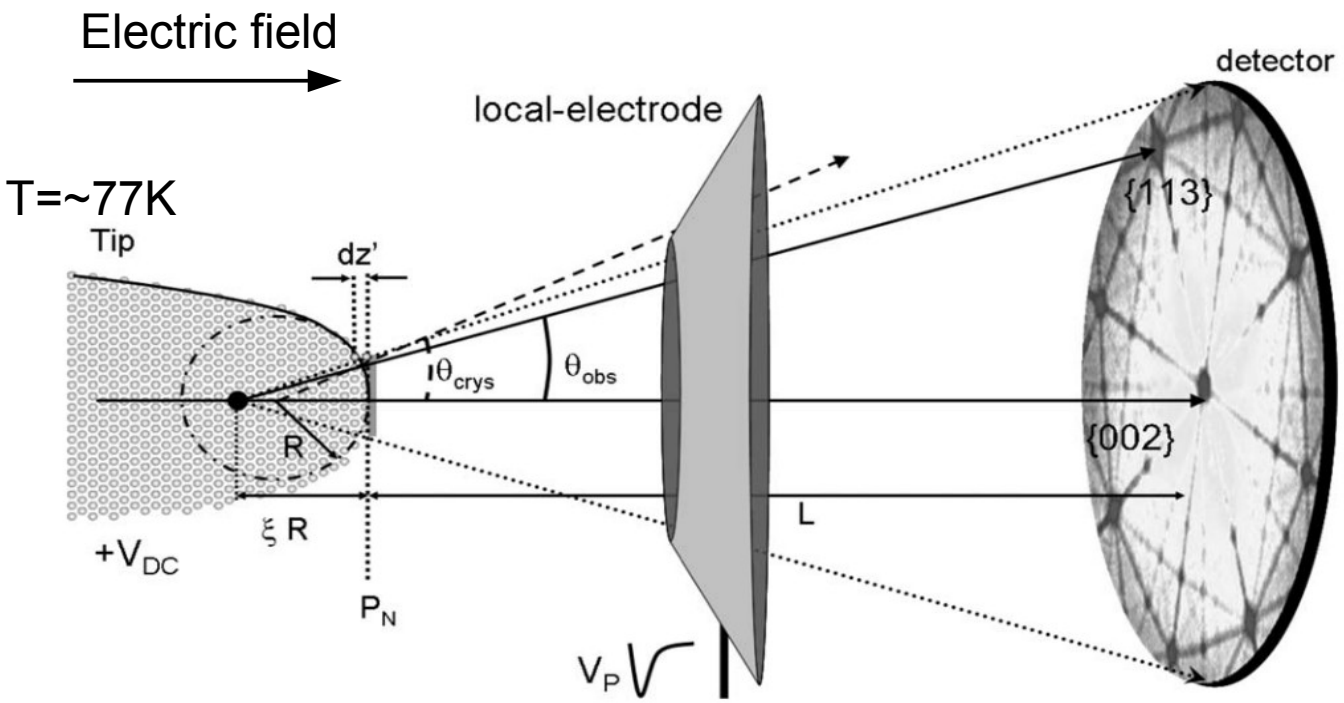
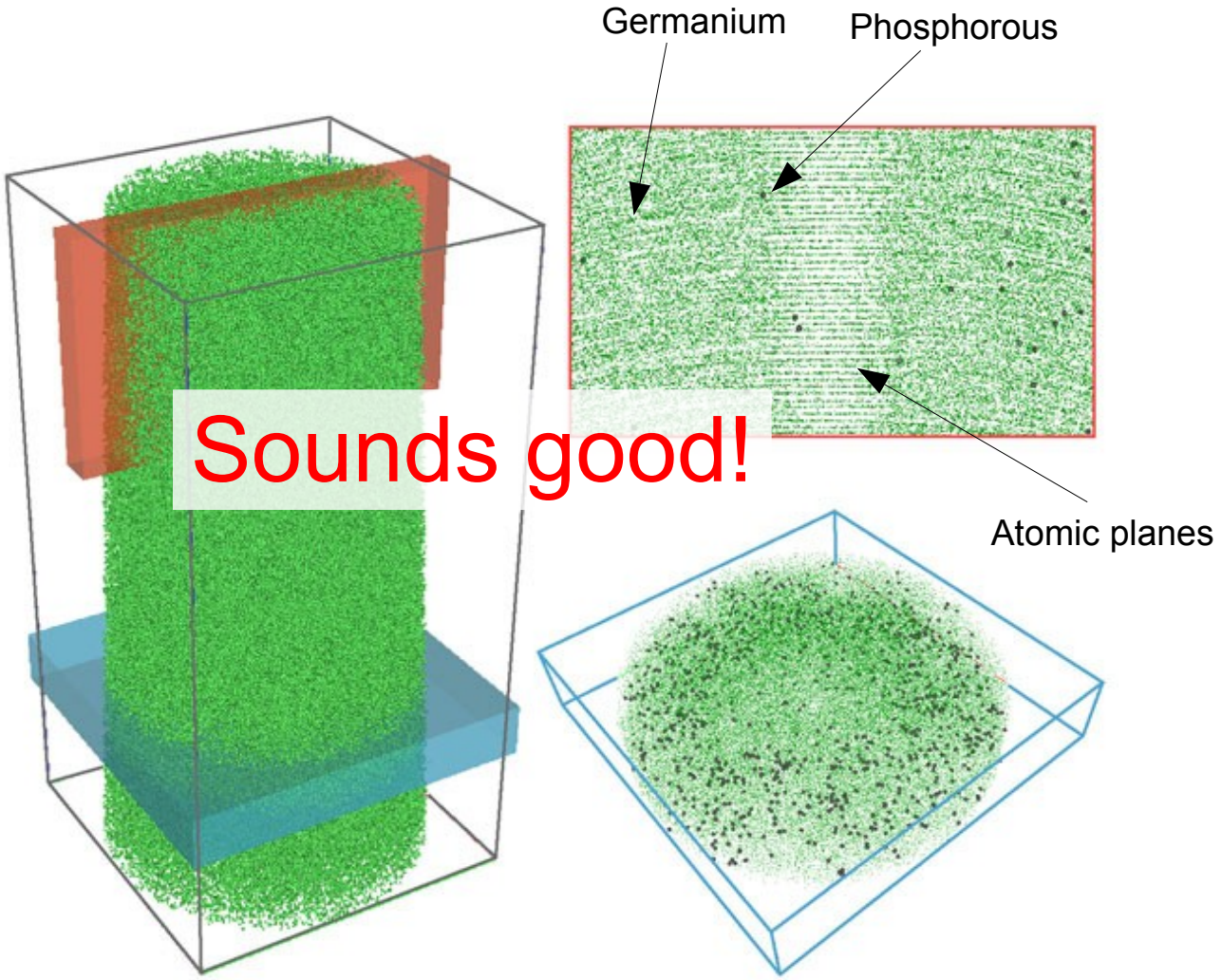


FIG. 1. Experimental setup of a modern atom probe.

(Gault 2009)

How it works



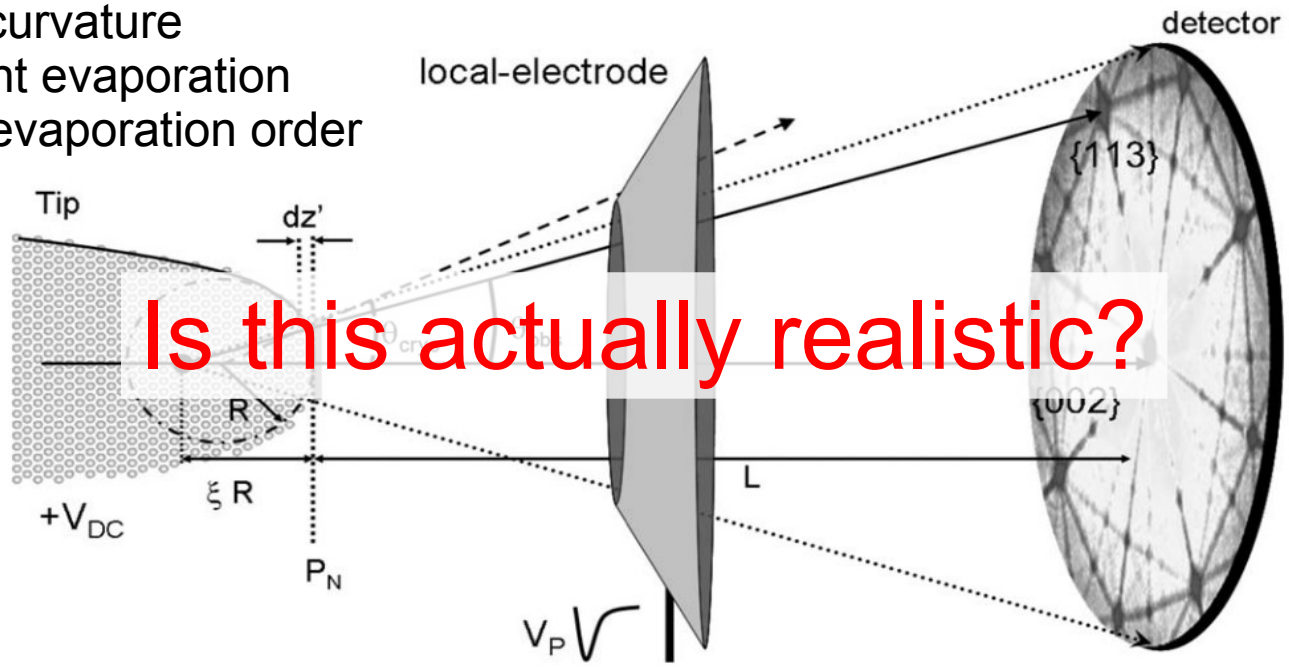
Sounds good!

(Robert R. McCormick School of Engineering and Applied Science)

A closer look at the “standard reconstruction model”

Assumptions:

- Assumed tip curvature
- Radial, straight evaporation
- Well-defined evaporation order

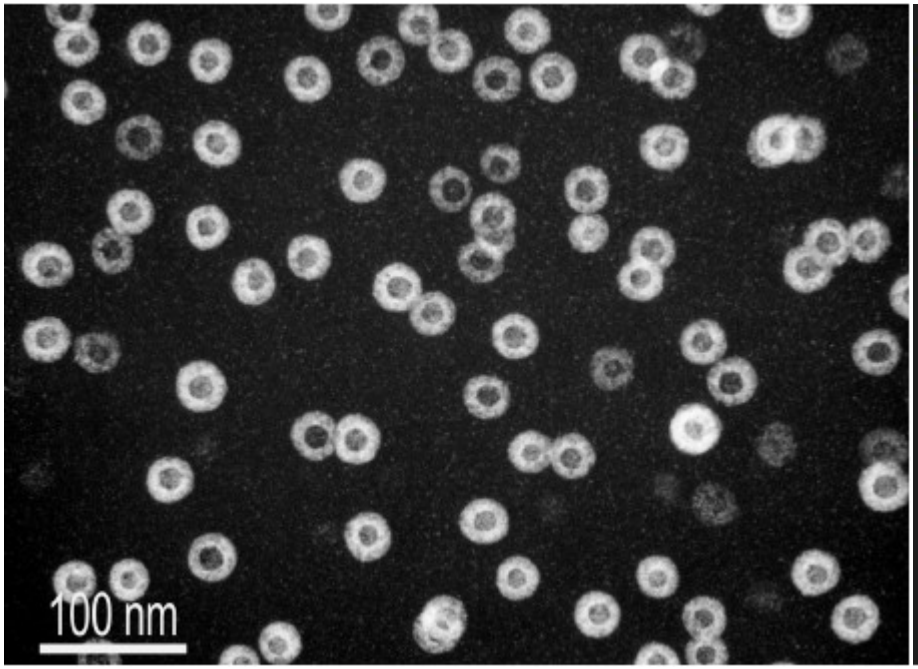


Is this actually realistic?

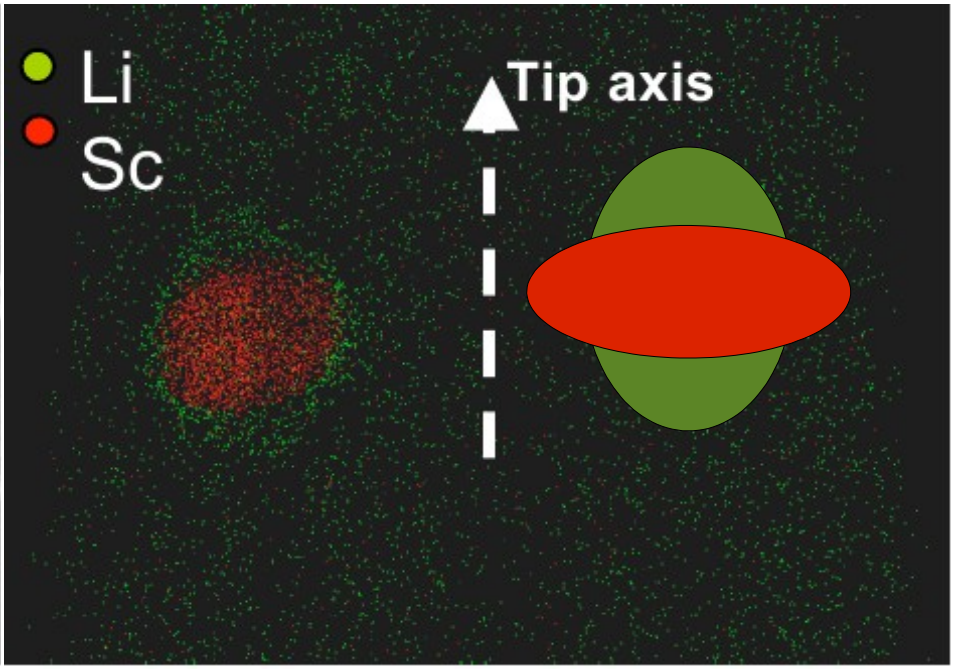
FIG. 1. Experimental setup of a modern atom probe.

Problem: Precipitates

Dark-field TEM



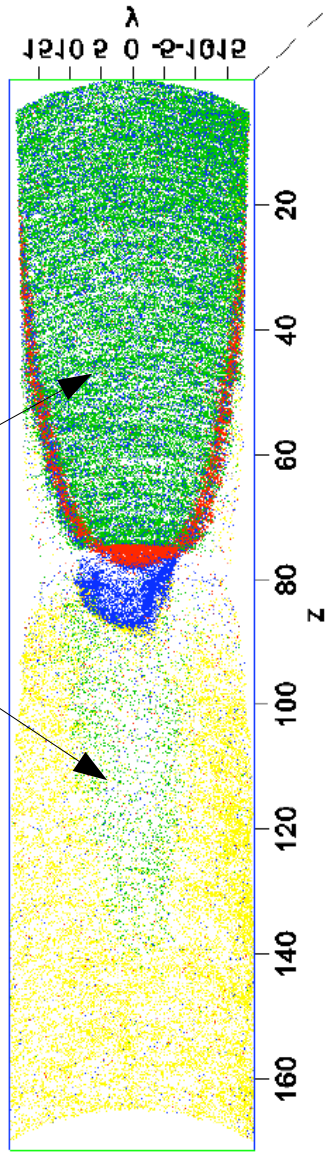
Atom Probe Tomography



Core/shell precipitates in Al–Li–Sc–Zr alloy (Marquis)

“Worst case scenario”

Should be on top of each other

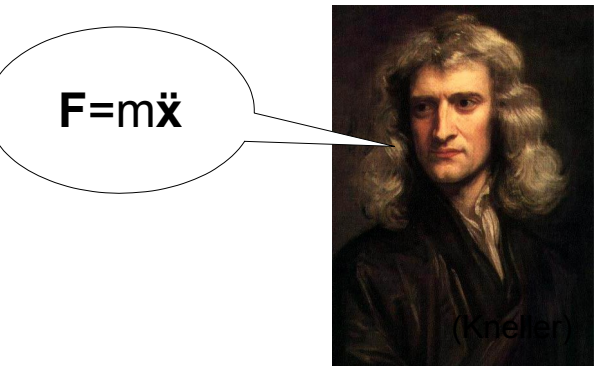


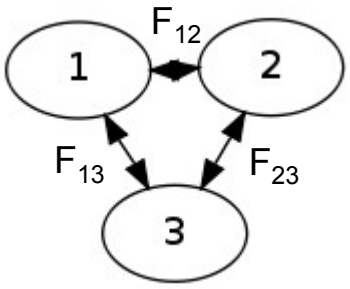
(Marquis)

Our goal

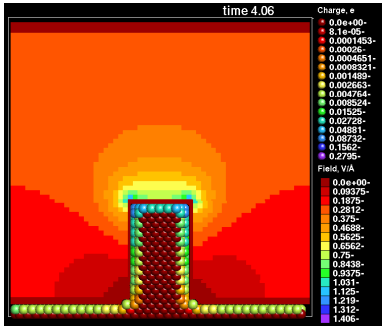
- Simulate the processes in APT to check the assumptions
- In the simulations we know the exact original sample shape and composition
    - These can be compared with what the reconstruction algorithms tell us it should look like
- Simulations performed using Molecular Dynamics to capture the dynamic evolution of the simulated sample
    - Previously other groups have used much simpler methods

Molecular Dynamics



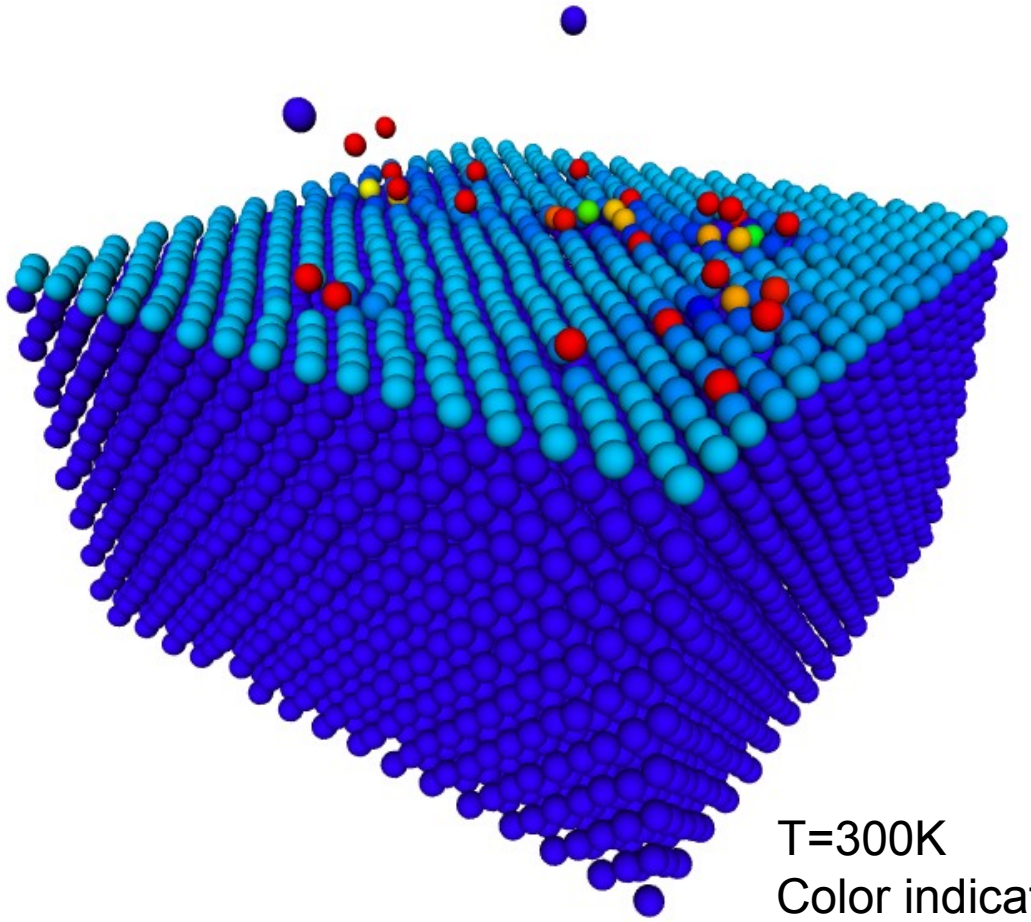


- Calculate forces acting on atoms, solve equations of motion
- Traditionally only inter-atomic interactions are included in MD
  - We also consider the forces due to the external electric field
  - Surface charge calculated using Gauss' law
  - (code also supports field emission heating but not used in APT simulations)
- Shape of the field depends locally on the sample geometry
  - Determined by solving Laplace's equation using



Simulating evaporation

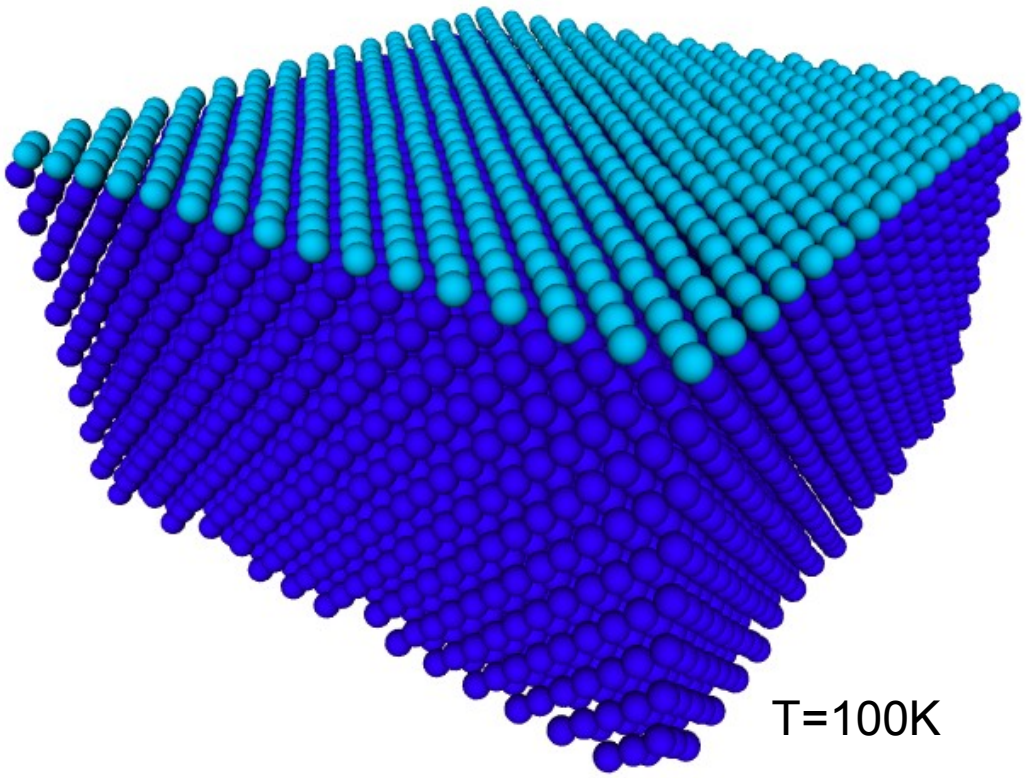
- In principle the hybrid ED&MD code is all that is needed to simulate field assisted evaporation



T=300K
Color indicates charge

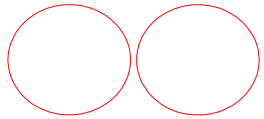
but...

- At low temperatures the evaporation probability decreases markedly

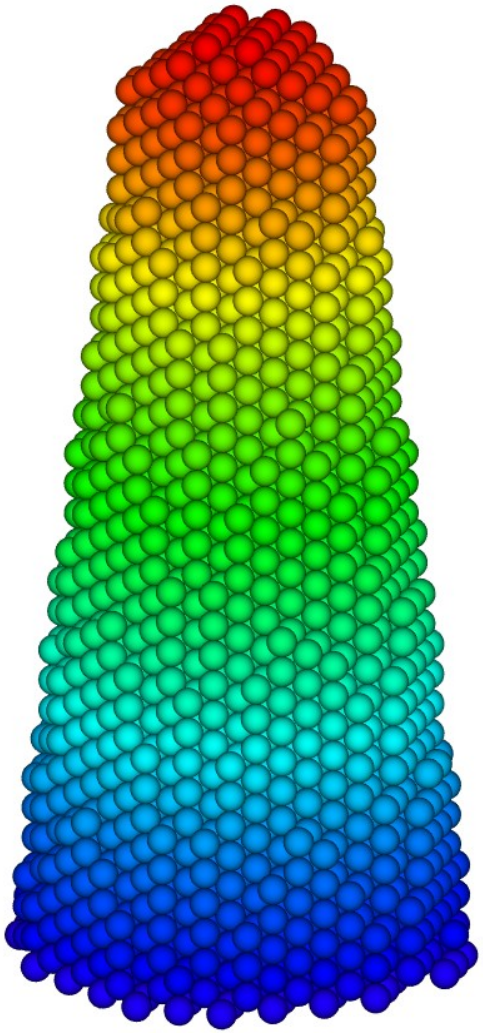


Simulating evaporation efficiently

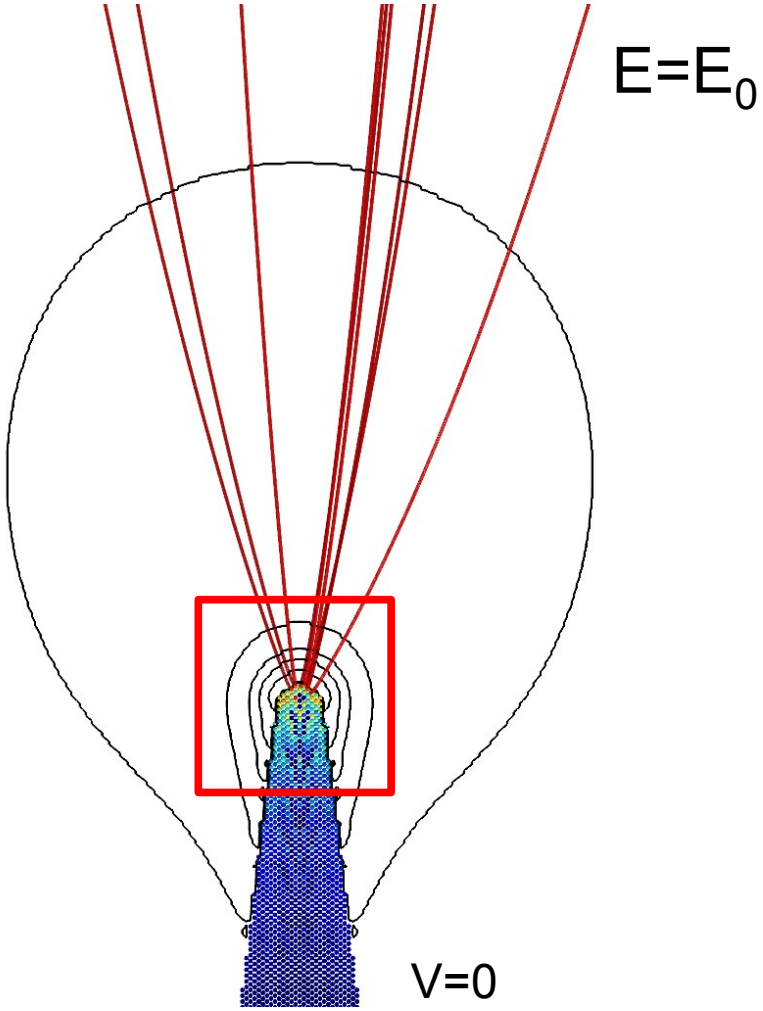
- Use a Monte Carlo step to pick atoms for evaporation
  - Probability
  - Evaporation Barrier $Q = Q(T, E_b, \Phi, U)$
  - Assume singly ionized state
    - Actually depends on the material
  - No multiples (one evaporation at a time)
    - Could be added later



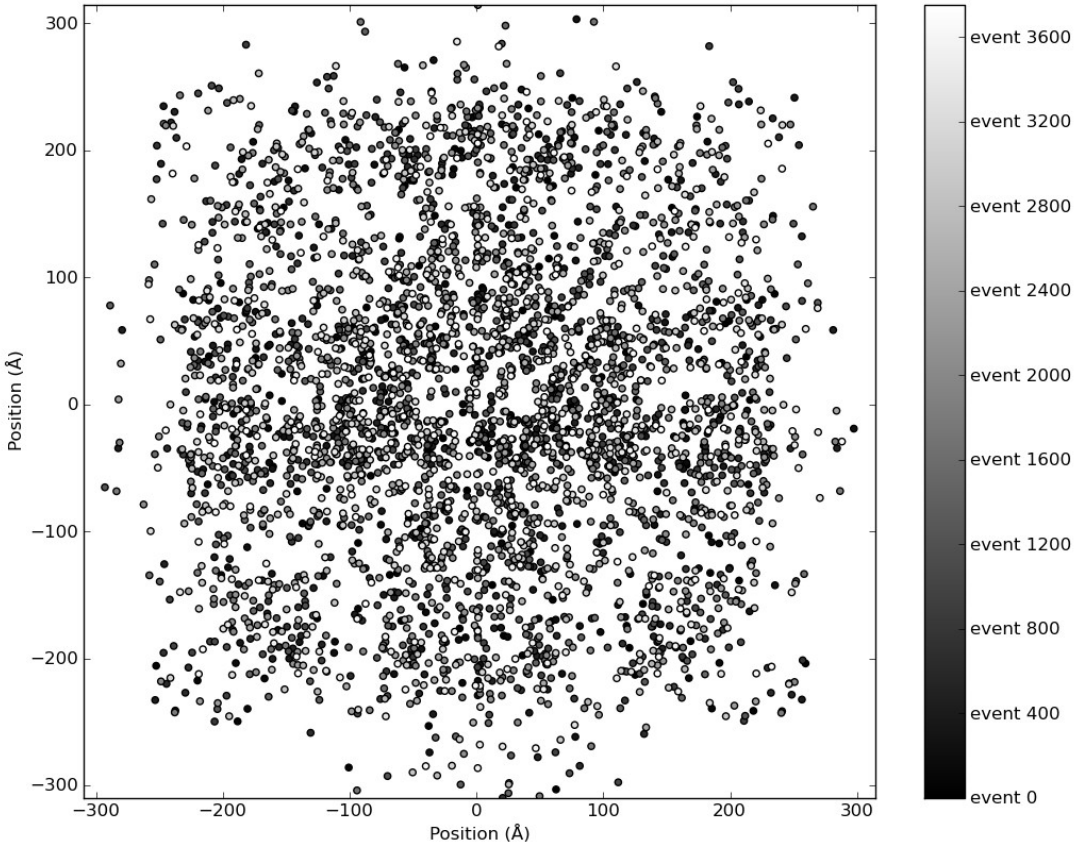
Reconstruction - original



Reconstruction - trajectories



Reconstruction – detector hits



Reconstruction – end result

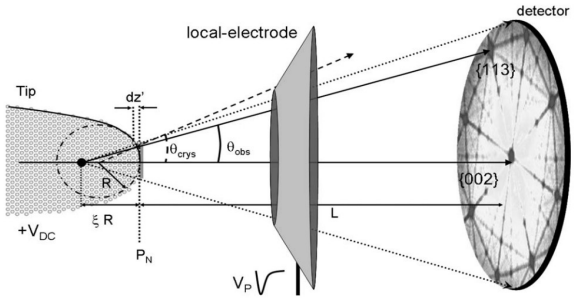
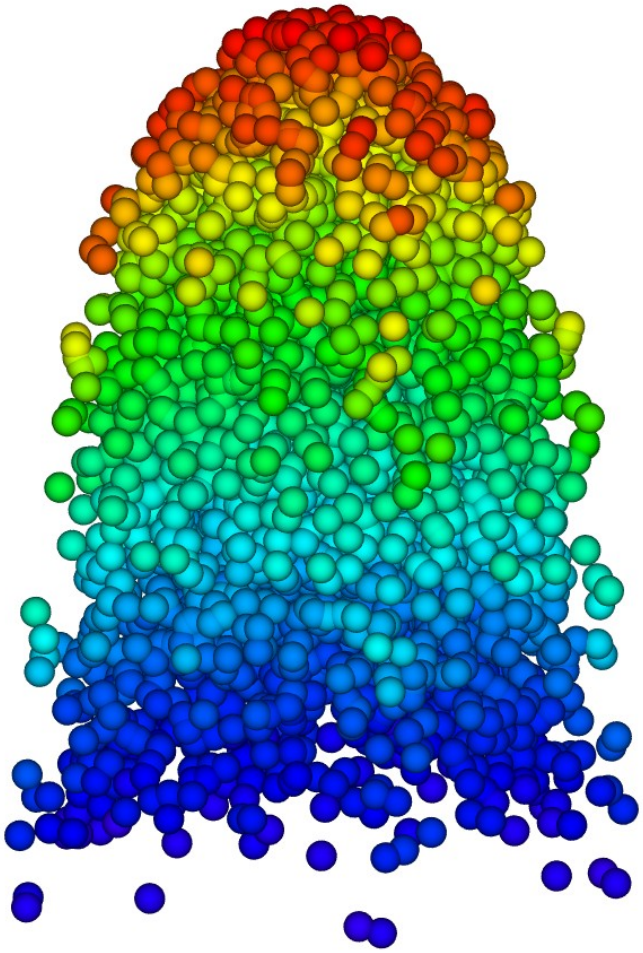
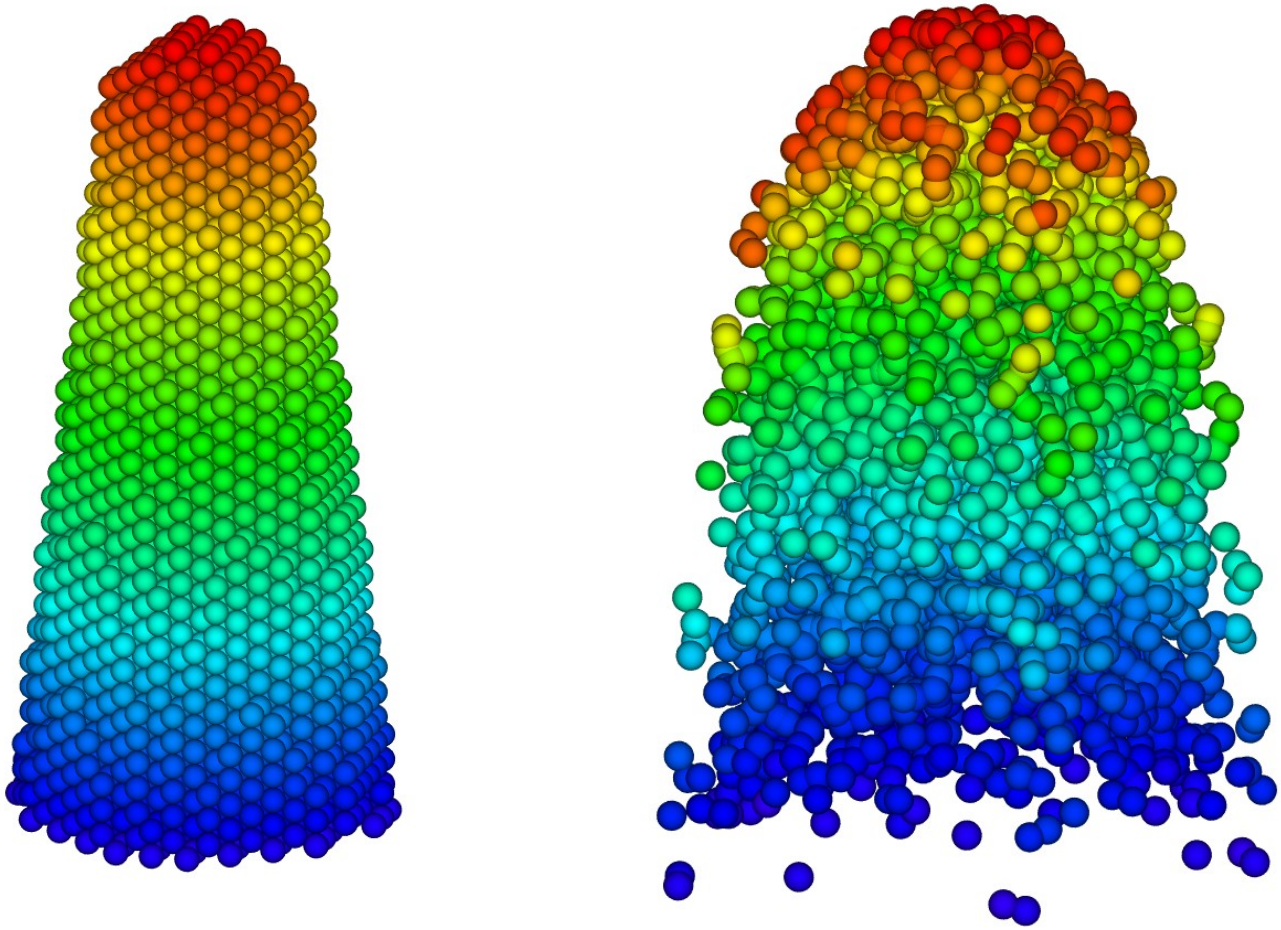


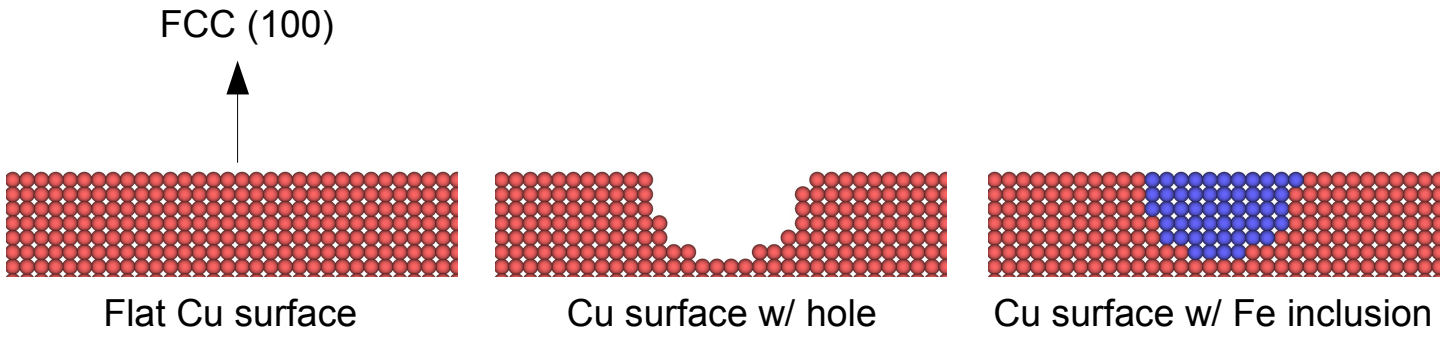
FIG. 1. Experimental setup of a modern atom probe.



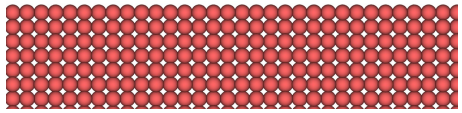
Reconstruction - comparison



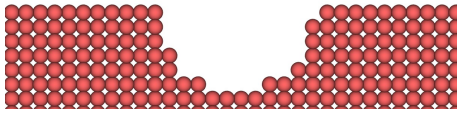
Effect of surface features



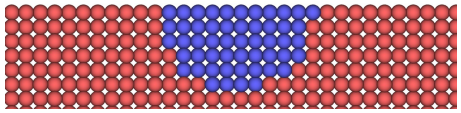
Some results



Flat Cu surface

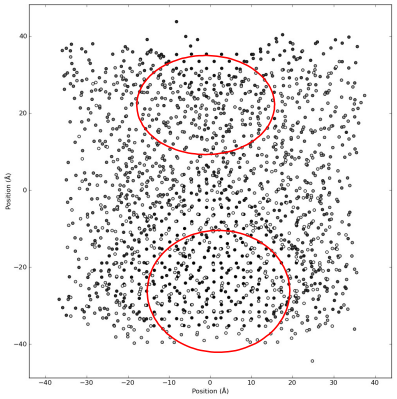


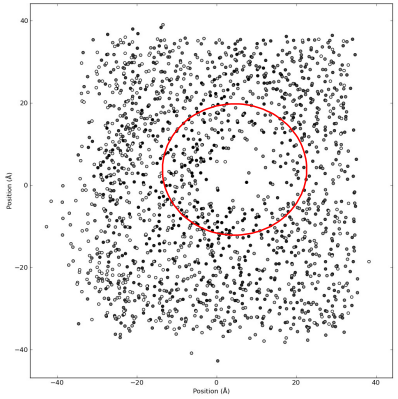
Cu surface w/ hole

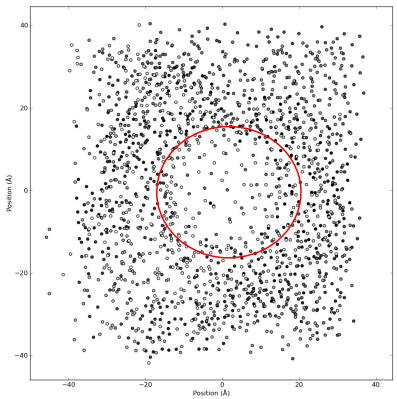


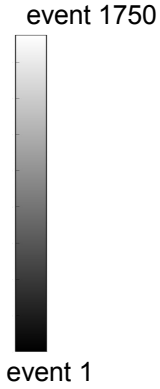
Cu surface w/ Fe inclusion

After 1750 events:

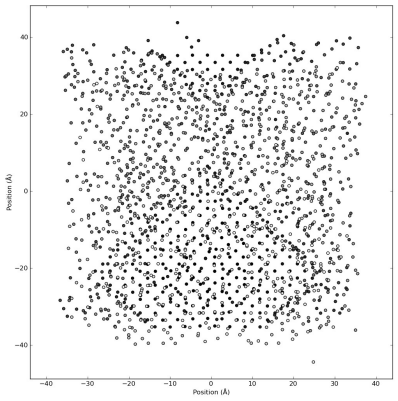


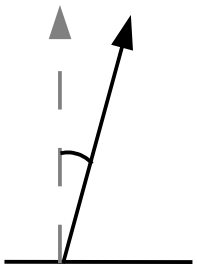


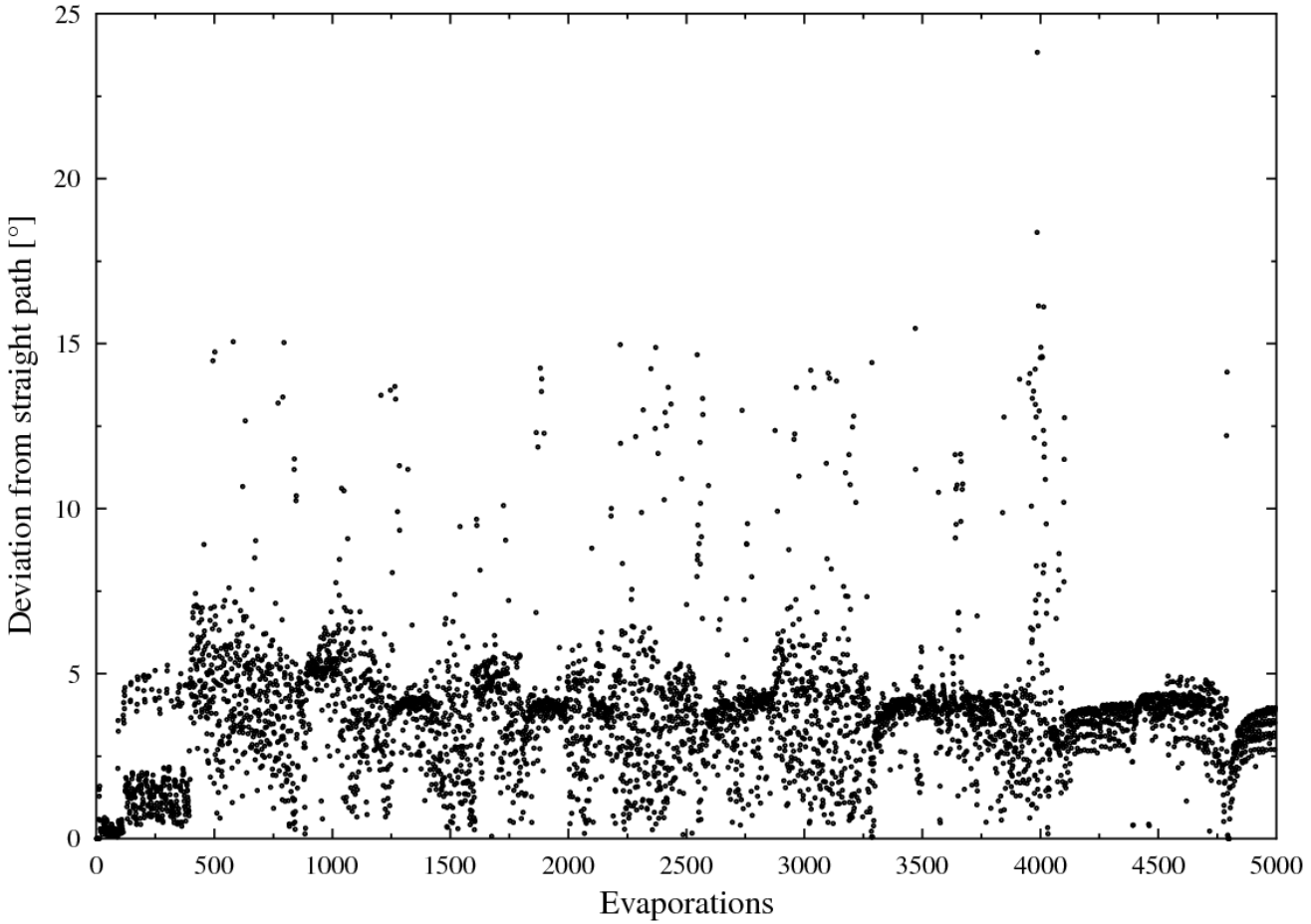




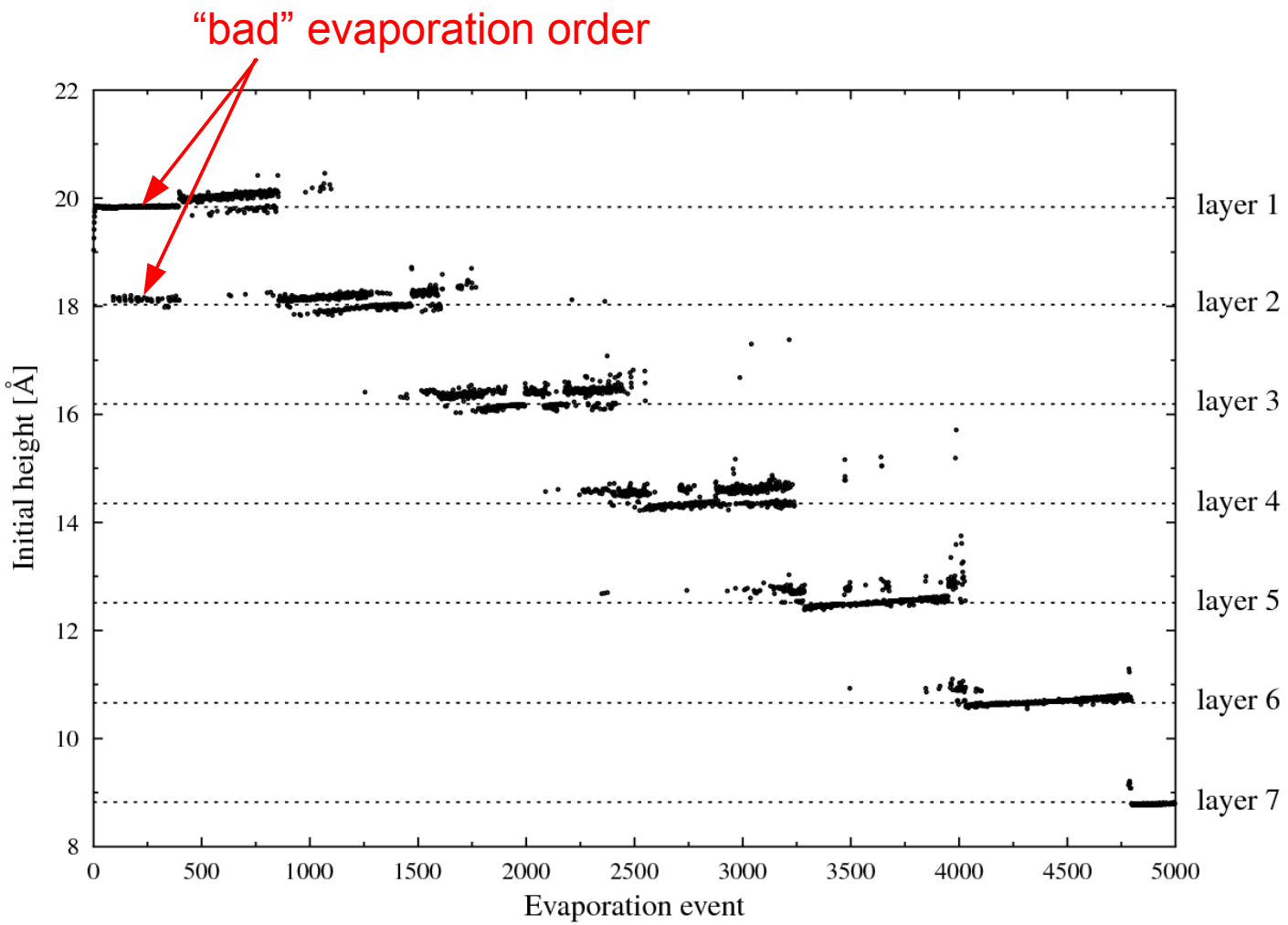
Pure copper surface: deviation



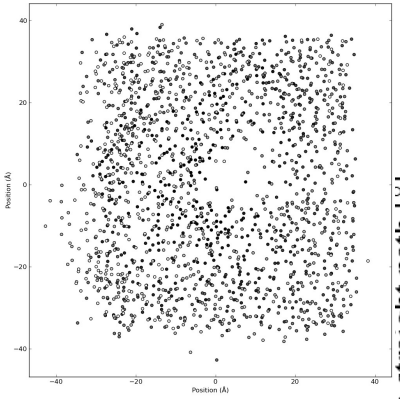


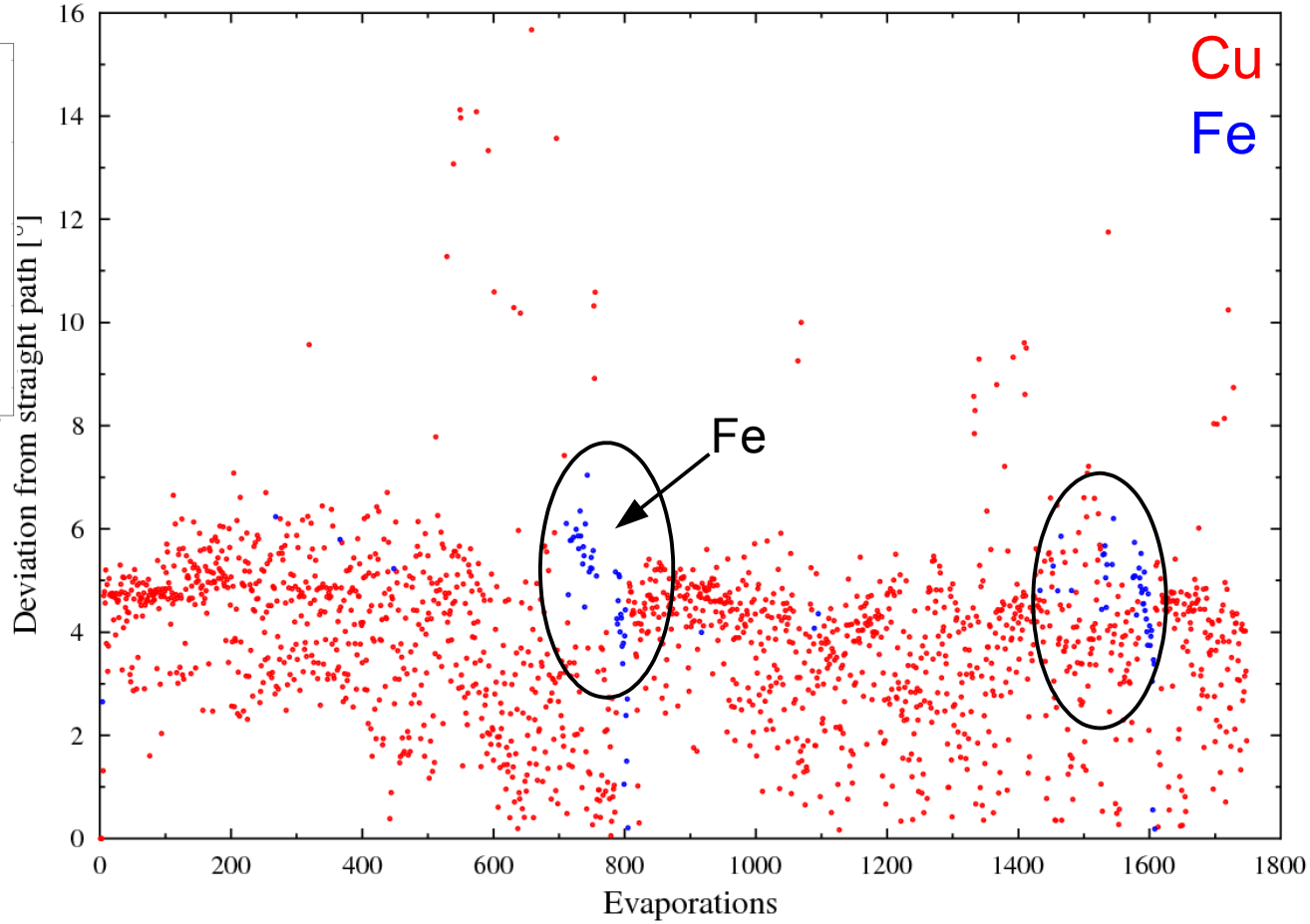


Pure copper: evaporation order

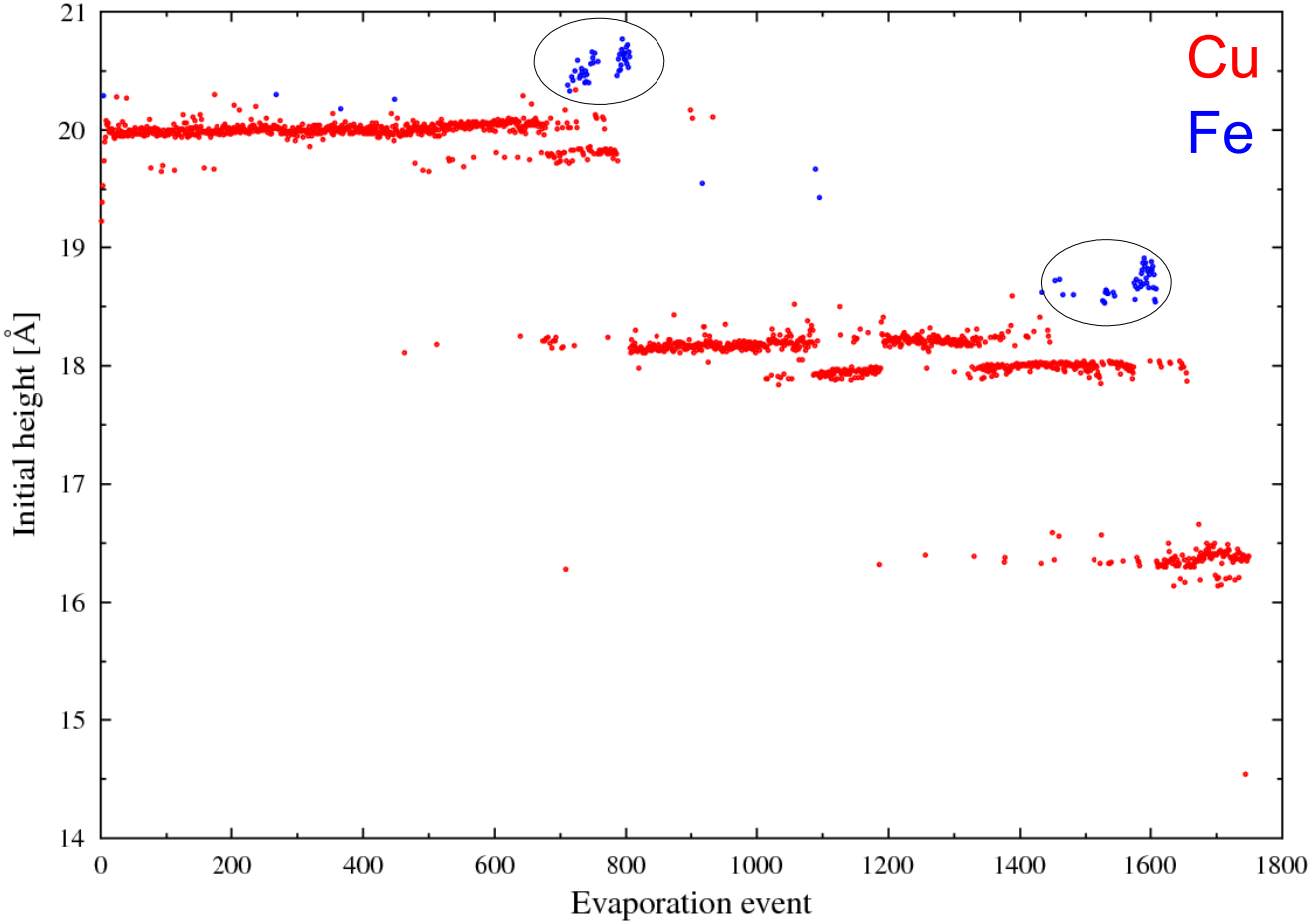


Inclusion: deviation

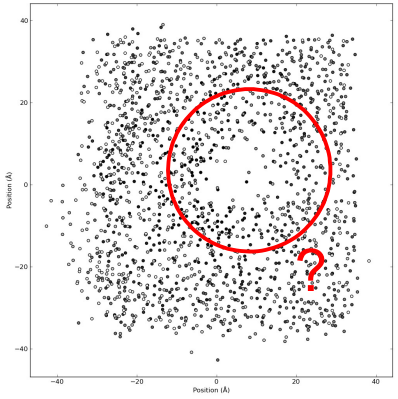


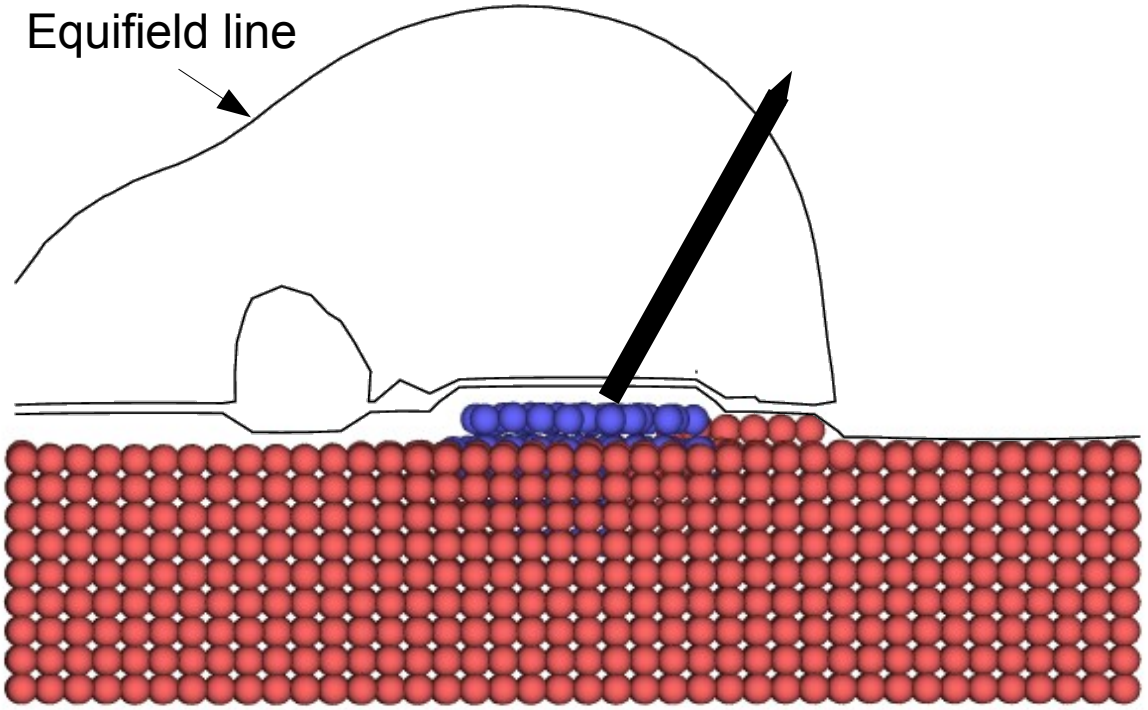


Inclusion: evaporation order

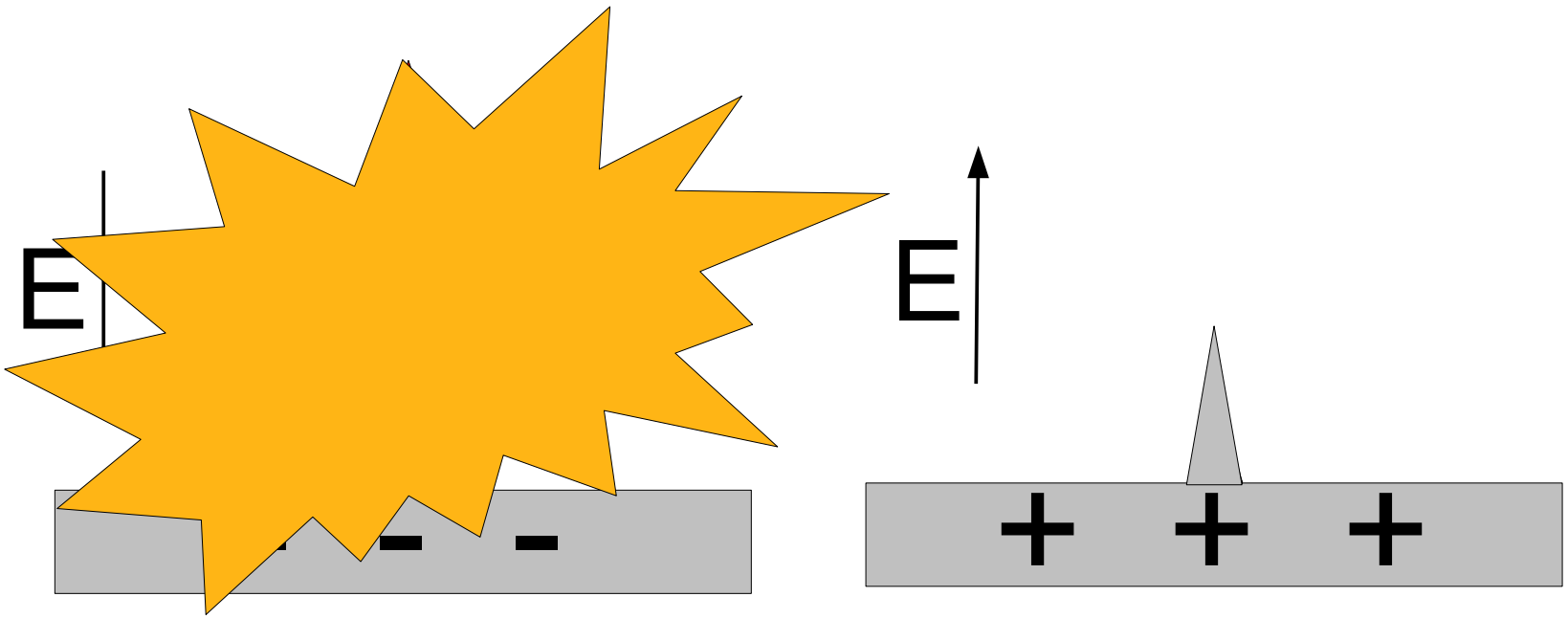


Inclusion: electric field distortion

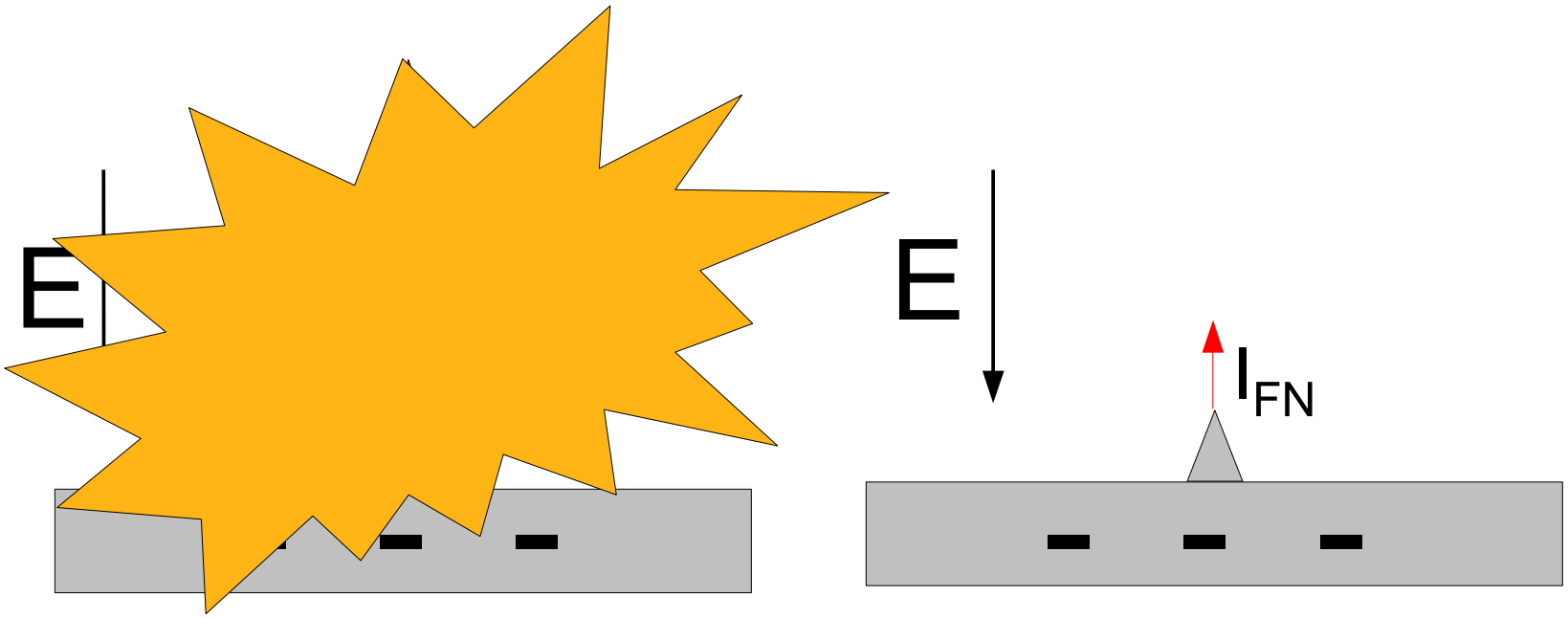




Back to breakdowns

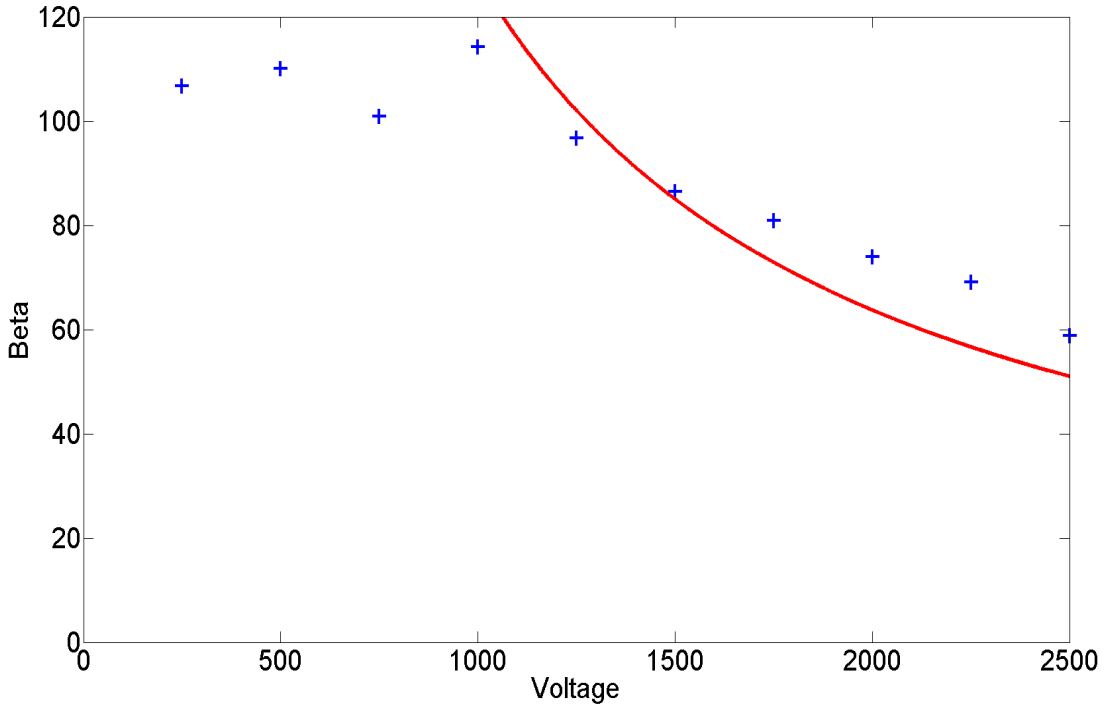


Application for breakdown prevention?



Possible surface treatment

- Tested at CERN DC setup
  - Very preliminary results
  - More tests to be performed later



(Nick Shipman)

Conclusions

- We have developed a new model to simulate field evaporation at low temperatures
- Reconstructing simulated specimen gives a reasonably good result
- Results show that changes in surface morphology affect ion trajectories
  - Deviations in trajectories
  - “Incorrect” evaporation order
- Field evaporating a surface may reduce breakdown probability

Outlook

- The method will be published soon
- Comparison of simulations with experiments
  - Collaboration with APT group at ETH Zürich
  - Need to make the results “compatible”

53rd International

IFES2012

MAY 21-25

Field Emission Symposium

HELSINGIN YLIOPISTO
HELSINGFORS UNIVERSITET
UNIVERSITY OF HELSINKI

What happened at IFES 2012?

- Not much about field emission
  - Renamed to APT&M for 2014 (Münster)
- Field emission and evaporation theory needed
  - But not many are working on it
  - Richard Forbes “promised” much improved FN equation soon
- Some groups working on effects of high electric fields on surfaces
  - But for APT, so no breakdowns
  - Changes in surface morphology
  - Calculation of surface charge