Metal surface evolution with and without an external electric field

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Outline

- Background: Tips
- Method: Kimocs (KMC)
- Results
  - Migration barrier calculations
  - Validation of the model
  - Stability of large tips
  - Tips under electric field
- Conclusions & outlook

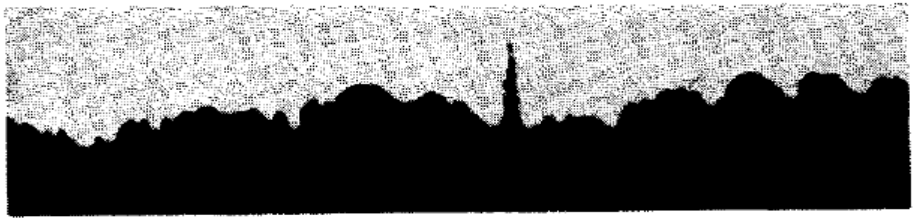
Nanotips

Field emission measurements suggests the existences of sharp nano-tips that would explain the ß factor in the Fowler-Nordheim equation.

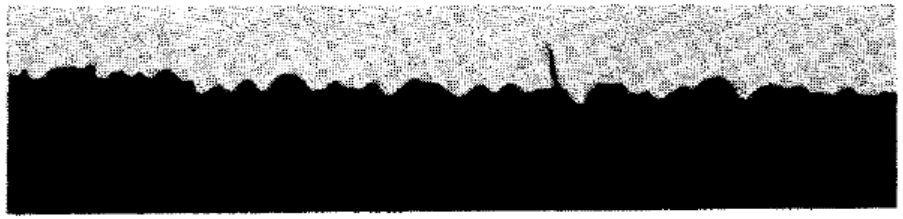
But tips are not likely to be seen after vacuum breakdowns

Observations of nanotips with aspect ratios of ~10 are rare, which raises the question: **How stable are nanotips?**

Nanotips



(a)



(b)

FIG. 4. Microprojections in the emission areas on optically polished cathode surfaces. (a) 304 stainless steel, (b) aluminum, magnification approximately ×2000.

~2 μm tips with an aspect ratio of ~10 were observed already 1963 on Cu and other metal surfaces by Little & Whitney (JAP), using transmission electron microscopy.

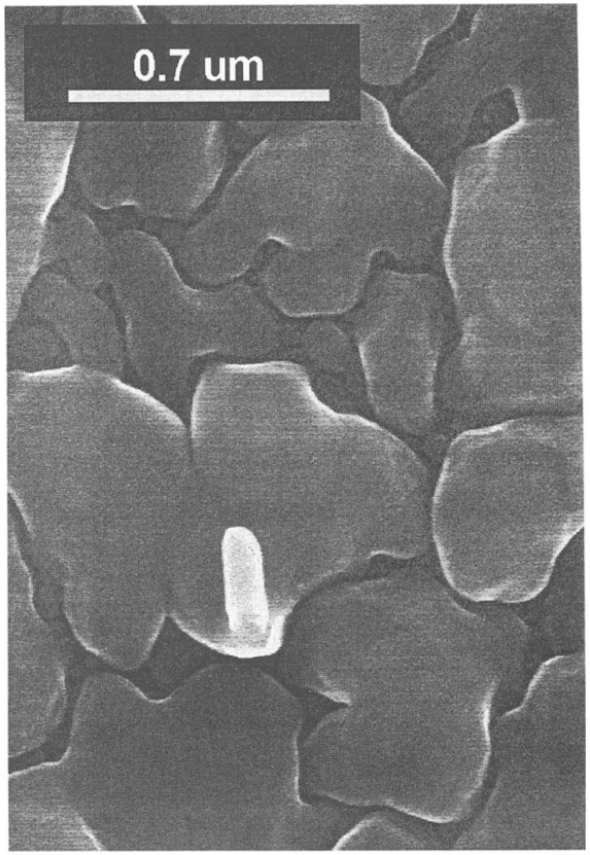
They used a field of 10 MV/m and a 10^{-5} Pa vacuum.

Nanotips

Copper tips with a radius <120 nm and height >300 nm, like the one in the SEM figure, have been found to be **stable for more than a month** at room temperature

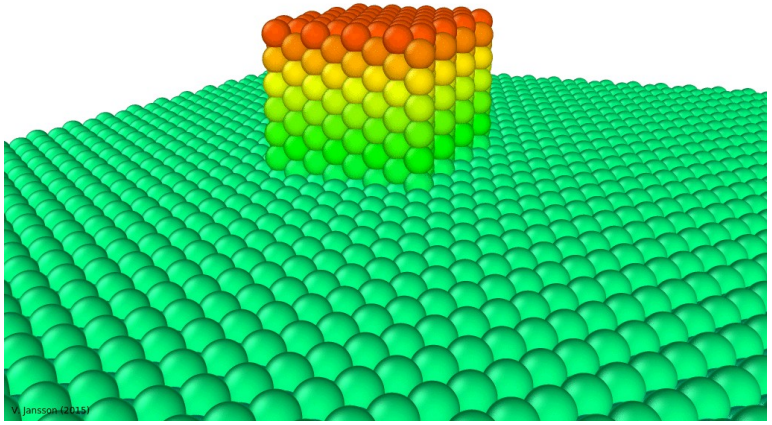
The tip was produced using metal organic chemical vapor deposition of Cu on quartz

In lack of good observations of tips, modelling can provide more insights.



[F. Atamny, A. Baker. Surf. Sci. (1995)]

Kinetic Monte Carlo (KMC)



- Simulation method for slow physical processes (nanoseconds – seconds for atomic processes)
- Thermally activated processes, such as atom jumps, have probability rates of the form

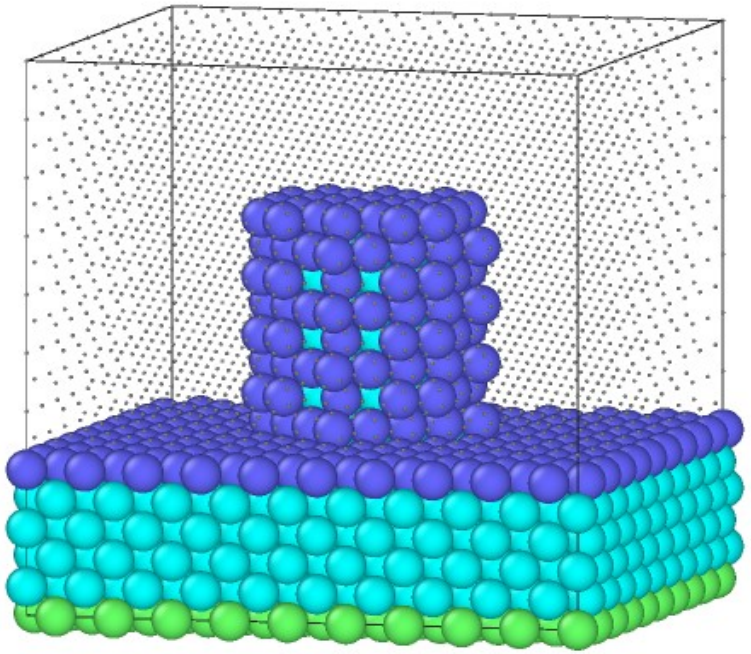
$$\Gamma = \nu \exp\left(\frac{-E_m}{k_B T}\right)$$

  where ν is the attempt frequency and E_m the migration (or activation) energy
- ν and E_m need to be known for all processes

Kimocs

A KMC code for the surface

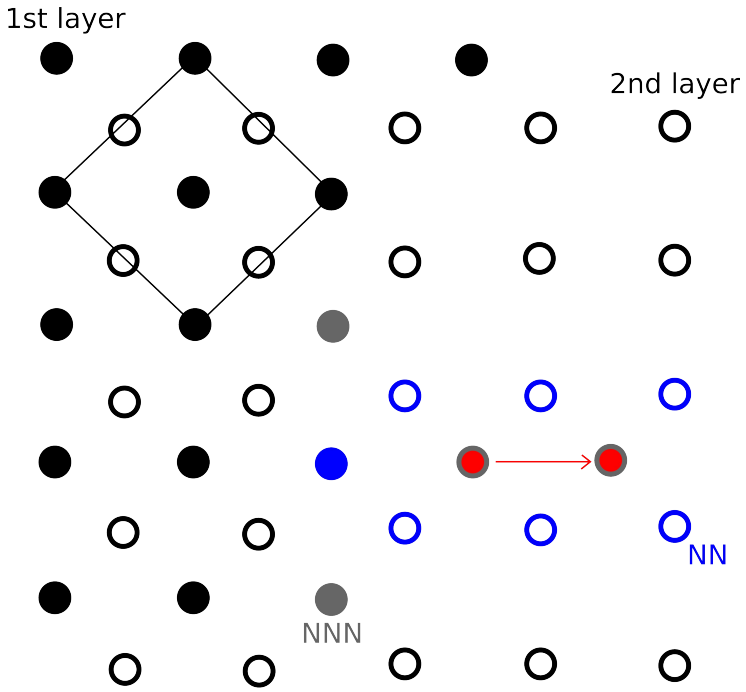
- Designed to simulate the surface evolution on the atomic scale
- Only surface atoms (blue) can migrate by jumping to vacant lattice sites on a rigid 3D lattice
- Bottom atoms (green) are usually fixed
- Different surfaces are possible: (100), (110) and (111), but not different grains
- Only fcc and bcc are implemented



Kimocs

A KMC code for the surface

(100) surface

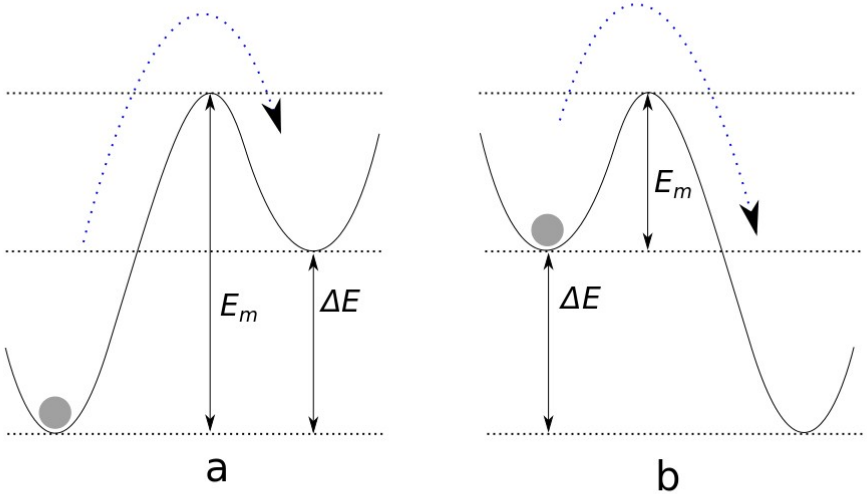


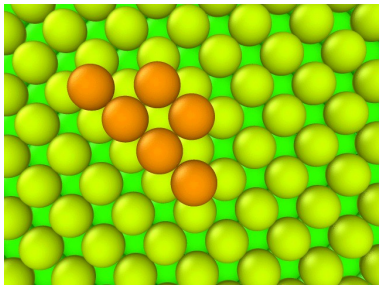
$E_m(5,3,5,1)$

- Atom jumps are characterized by
  - The number of nearest neighbour (1nn) atoms
  - The 2nd nearest neighbour (2nn) atoms

  of the initial and final lattice sites
- E_m for all processes are calculated with Molecular Dynamics

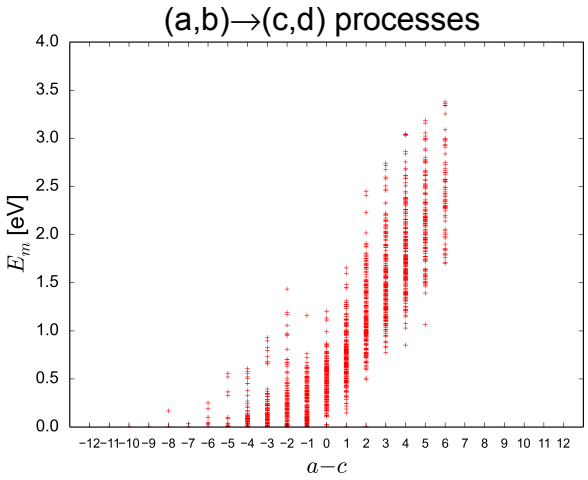
Calculations of the migration energies, E_m





(6,2)→(7,2)

- E_m for a process depends on the local atom configuration and can be described as (1nn,2nn)→(1nn,2nn)
- Thousand of configurations has to be considered
- The Molecular Dynamics method Nudged Elastic Band (NEB) is used



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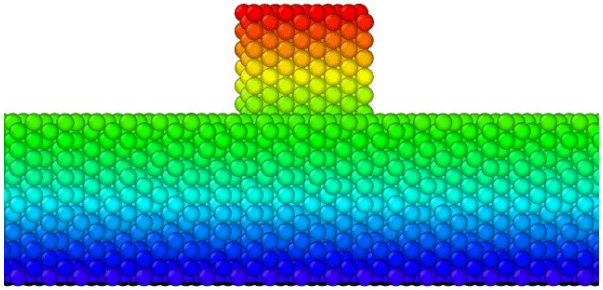
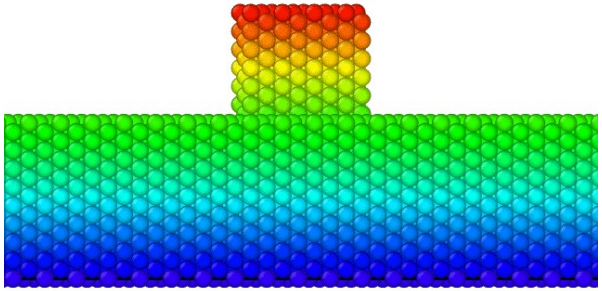
The attempt frequency ν

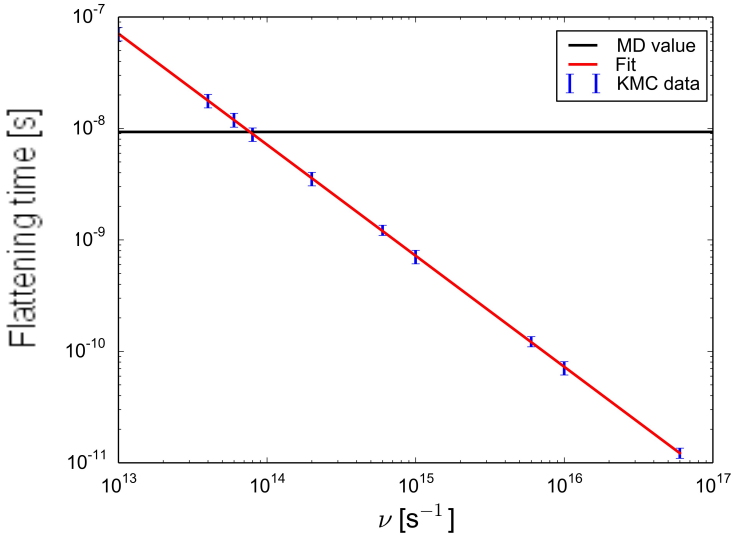
MD



KMC

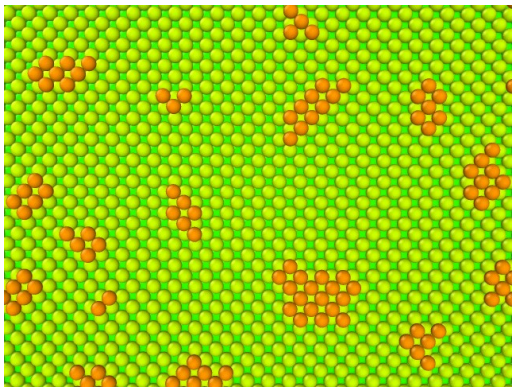


- Since all processes are atom jumps, ν can be considered a constant near to the Debye frequency of Cu, $4.5 \cdot 10^{13}$ s^{-1}
- Our value $\nu = 7 \cdot 10^{13}$ s^{-1} is obtained by fitting to MD simulation results of the Cu tip flattening proces

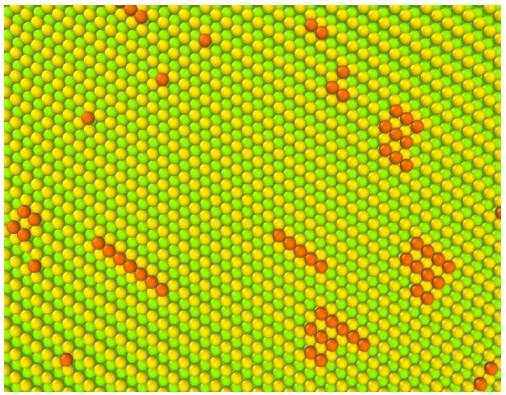


(100), (110) and (111) surfaces

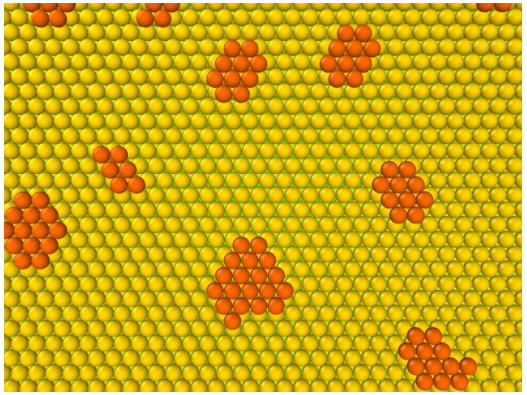
Kimocs simulations: Adatom islands



(100)



(110)



(111)

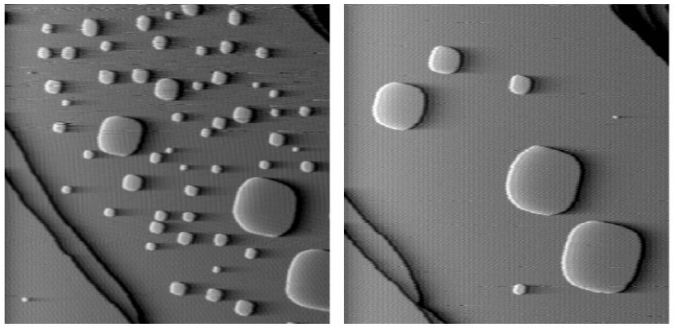
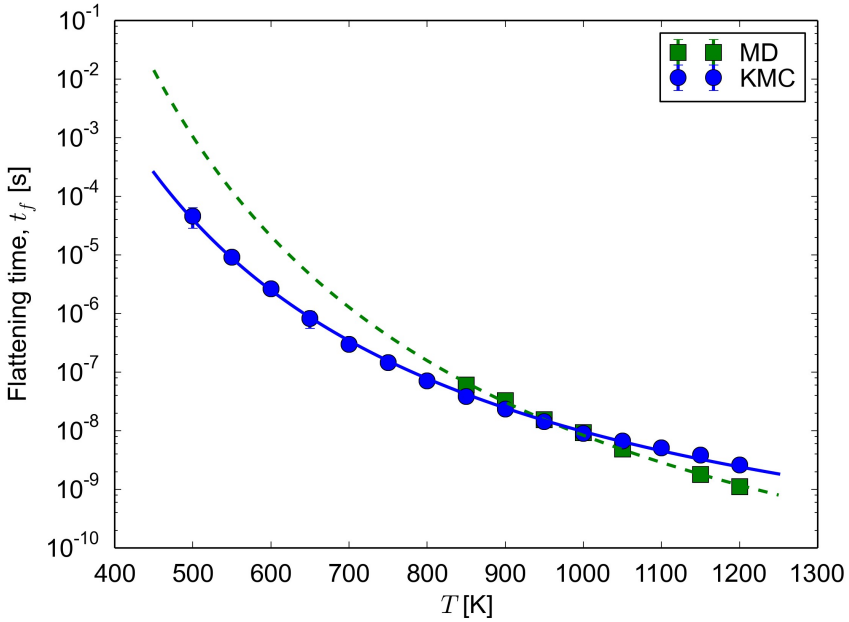


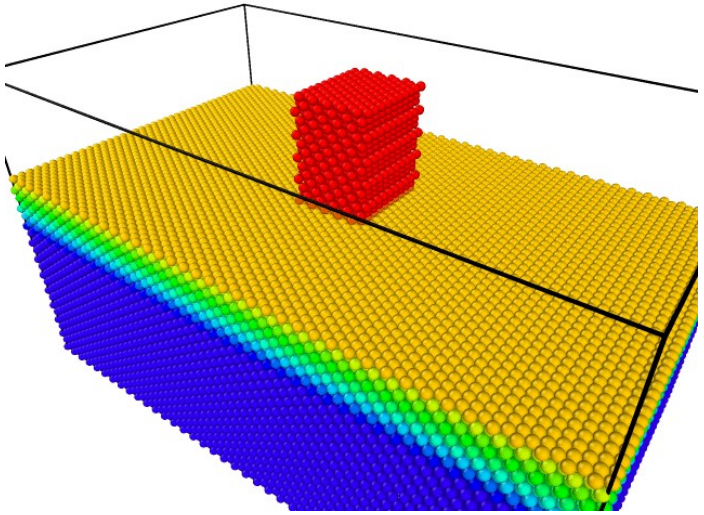
FIG. 2. Two 300 nm × 300 nm STM images, separated in time by 20 000 s, showing island ripening on Cu(001) at 343 K.

[J.B. Hannon et al. PRL 1997]

Tip flattening: KMC vs MD

Flattening of a [110] tip at different T

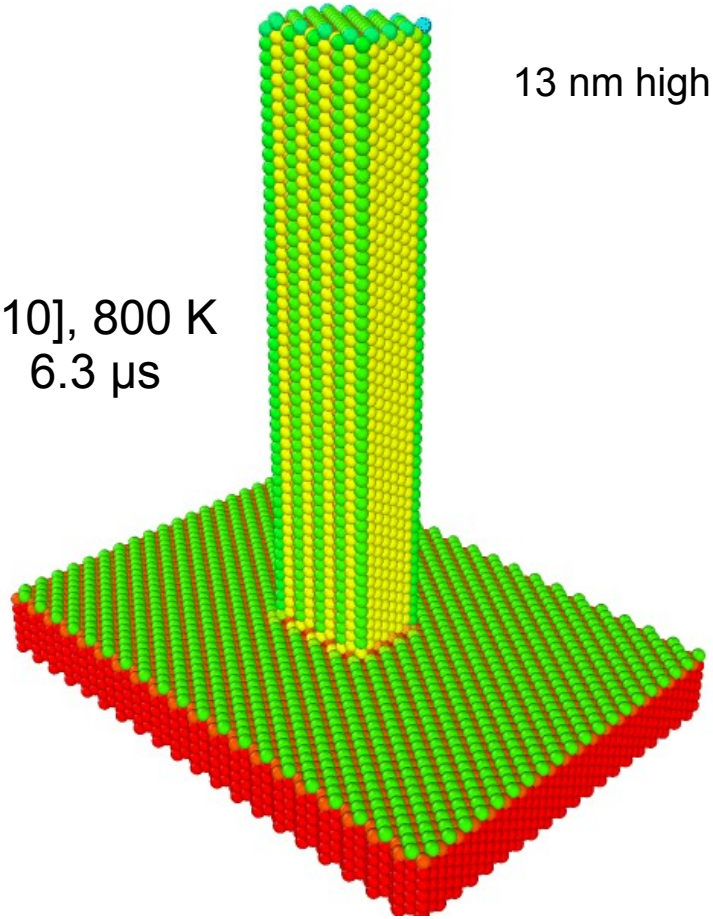




- Good agreement at 850—1150 K
- Strong temperature dependence
- KMC is ~100 times faster than MD

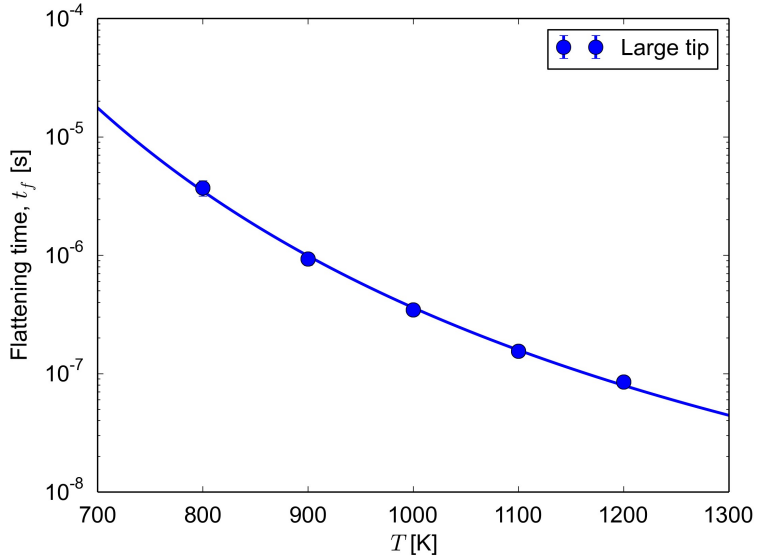
Stability of large tips

Kimocs simulations



13 nm high

[110], 800 K
6.3 μs



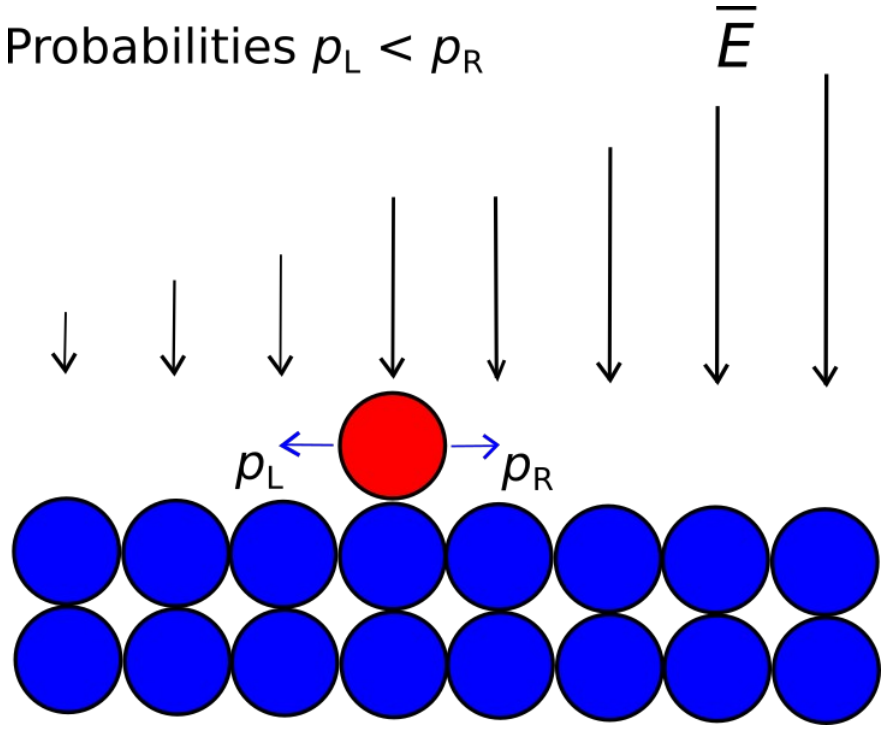
- <110> tips are the most stable ones
- At 300 K, no change was seen after 10 μs
- Extrapolation gives a flattening time of 3.1 h at 300 K

http://arxiv.org/abs/1508.06870 Submitted to PRB

The effect of electric fields

- The Helmod code has now been integrated with Kimocs for the calculation of field and charges
- Helmod is developed by F. Djurabekova and S. Parviainen et al., and has successfully been used in MD before
- Field is calculated by solving the Laplace equation (no space charge)
- Surface charges given by Gauss' law

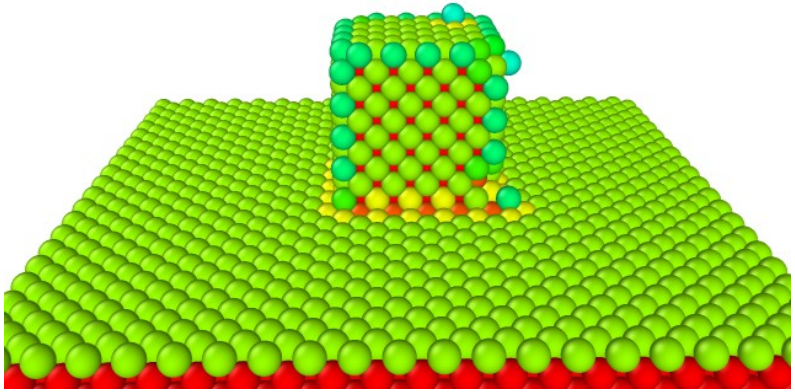
The effect of the electic field



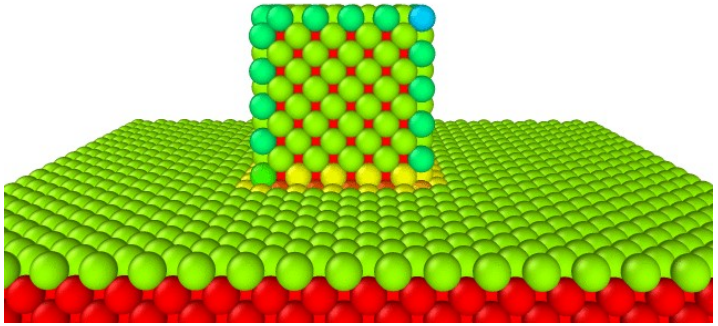
- In KMC, the migration barriers are lowered by the field: $\Delta E_m \sim qEd$. *(charge q, field E and jump distance d)*
- The diffusion becomes enhanced and biased

KMC with electric fields

Perfect cube after 155 ns in 300 K



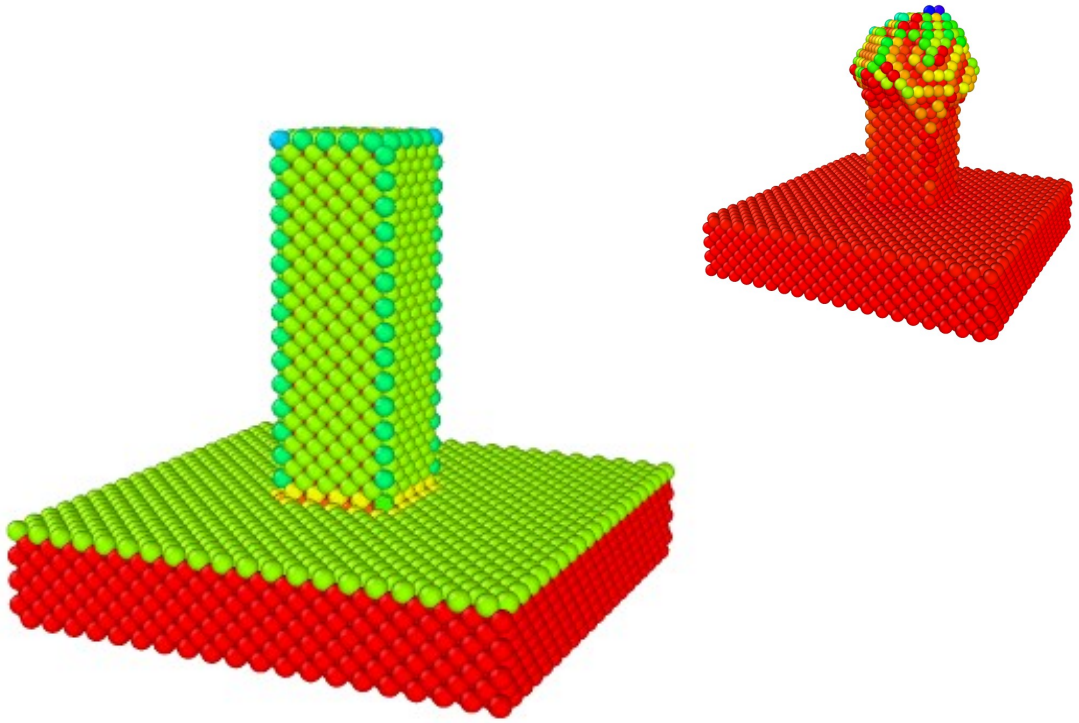
Same with a 1 GV/m gradient



KMC with electric fields

Charges

- 10 GV/m gradient
- T = 300 K
- 49 μs



Conclusions

- Our KMC surface model compares well with MD for Cu
  - The model also works for Fe and W (Au in progress)
- Cu tips with [110] orientation can be stable for hours at room temperature
- The tip flattening rate speed up with several orders of magnitude with higher temperatures
- We have a first implementation of the electric field into the KMC model for surface atom diffusion

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Cu(100), 5.5 ps, 700 K

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