Long-term surface evolution models for accelerator materials

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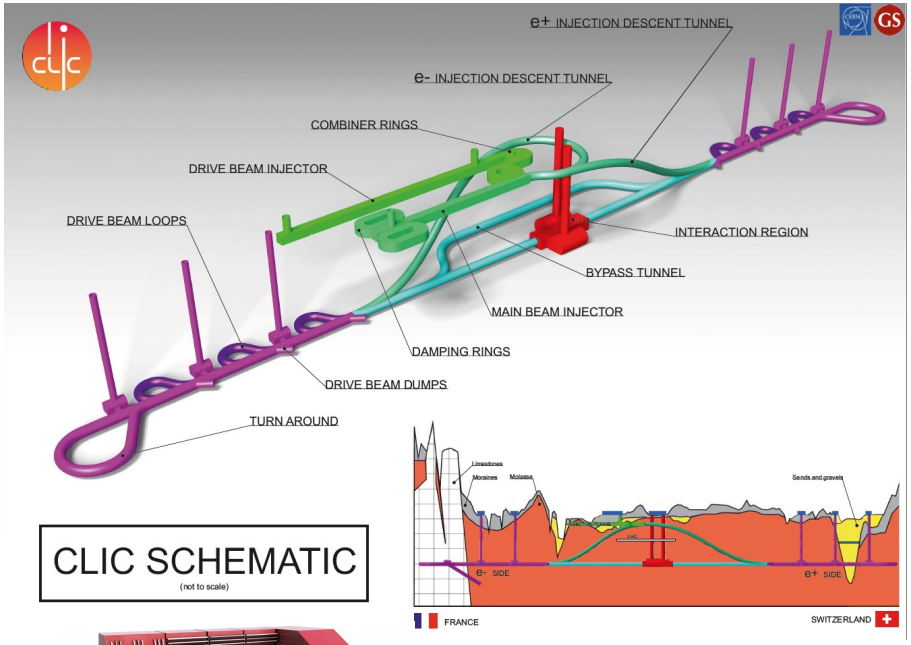
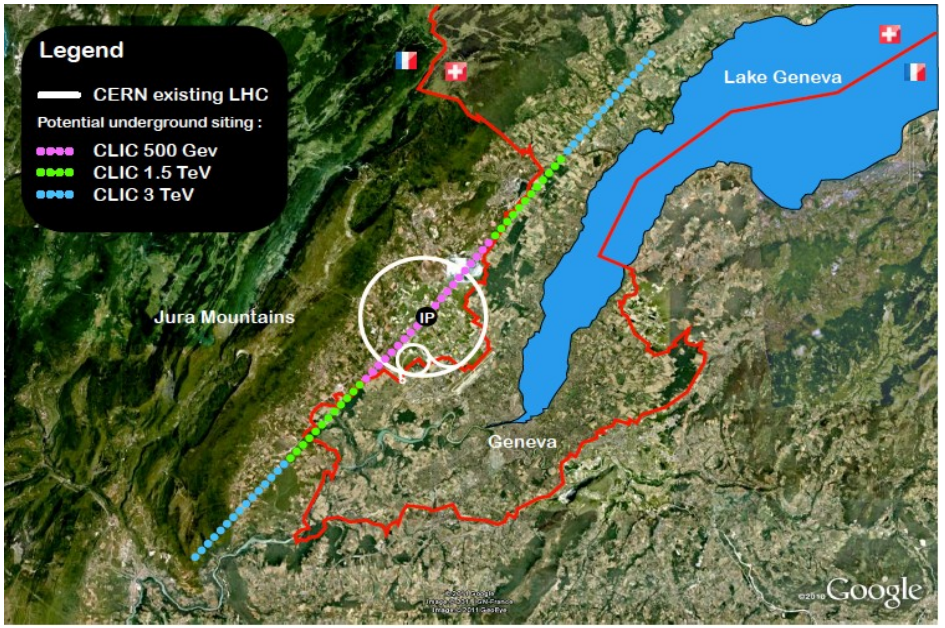
Outline

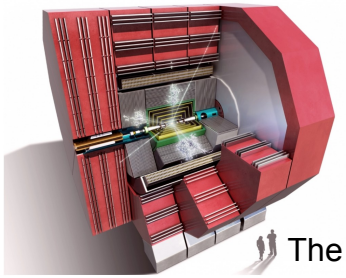
- Background:
  - CLIC
  - Vacuum arcs
- Method: Kimocs (KMC)
- Results
  - Migration barrier calculations
  - Validation of the model
  - Stability of large tips
- Conclusions & outlook

The Compact Linear Collider (CLIC)



CLIC SCHEMATIC
(not to scale)





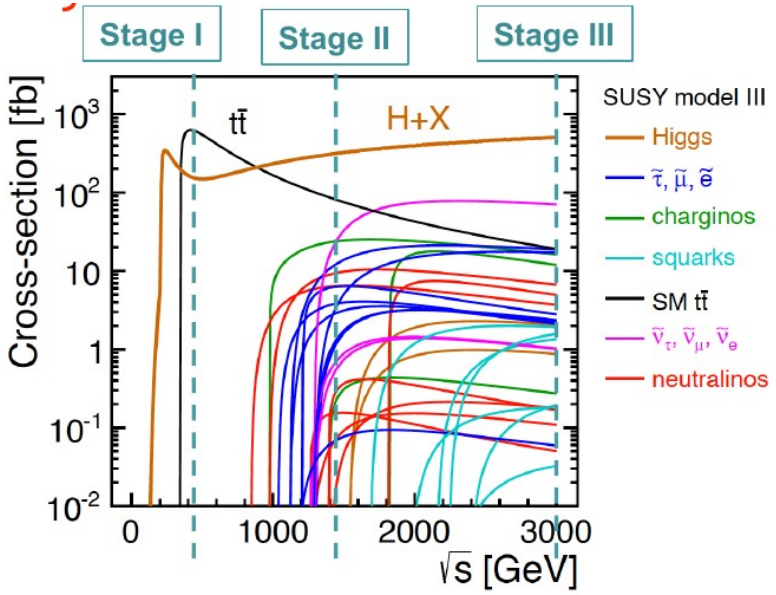
The detector

- Electron-positron collider
- Centre-of-mass energy: 380 GeV – ~3 TeV
- Length:10—50 km
- Construction decision 2018-2019

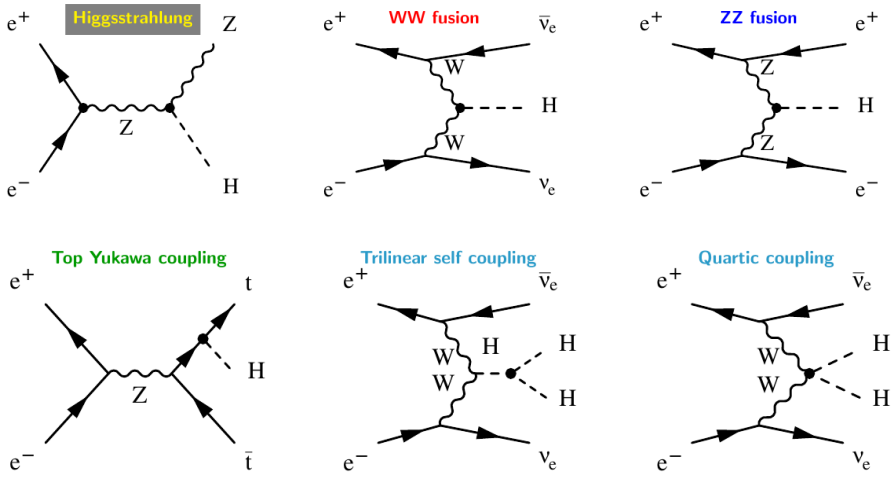
CLIC: particle physics point-of-view

The three stages of CLIC

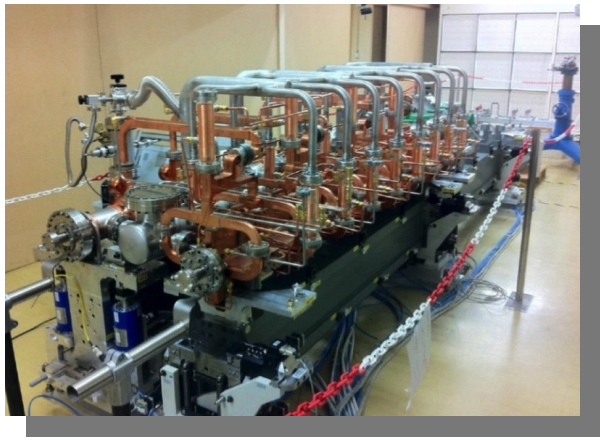
- Stage I: 380 GeV, 500 fb^{-1} (Higgs, top)
- Stage II: ~1.5 TeV, 1.5 ab^{-1} (Higgs, gauginos, sleptons)
- Stage III: ~3 TeV, 2 ab^{-1} (Higgs, squarks,...?)



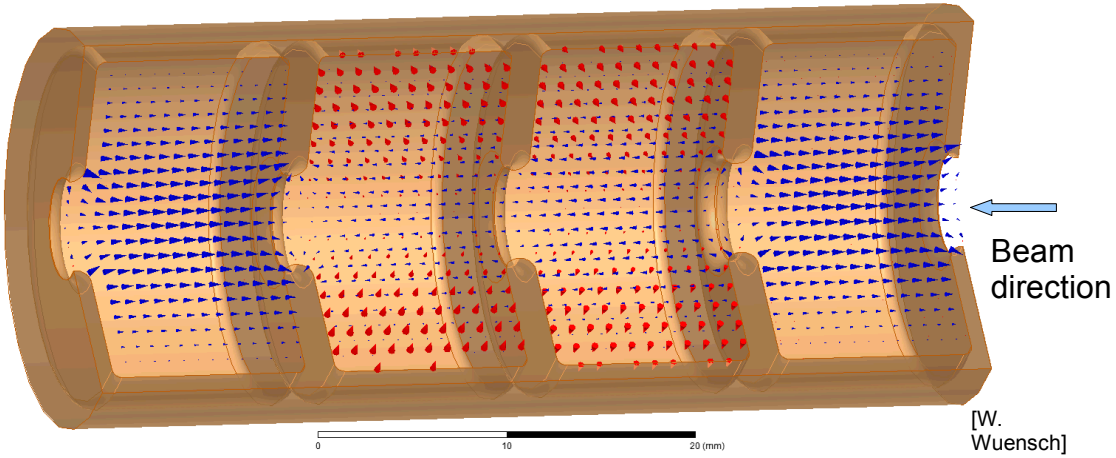
Higgs processes of interest for CLIC



CLIC: the accelerating structures

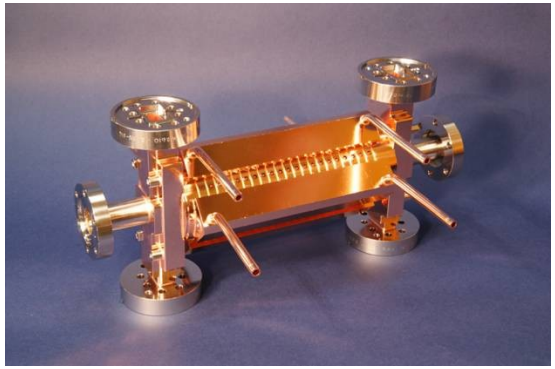


CLIC test model at CERN

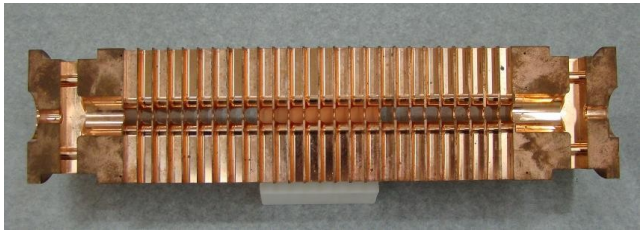


[W. Wuensch]

100–300 MV/m accelerating electromagnetic fields

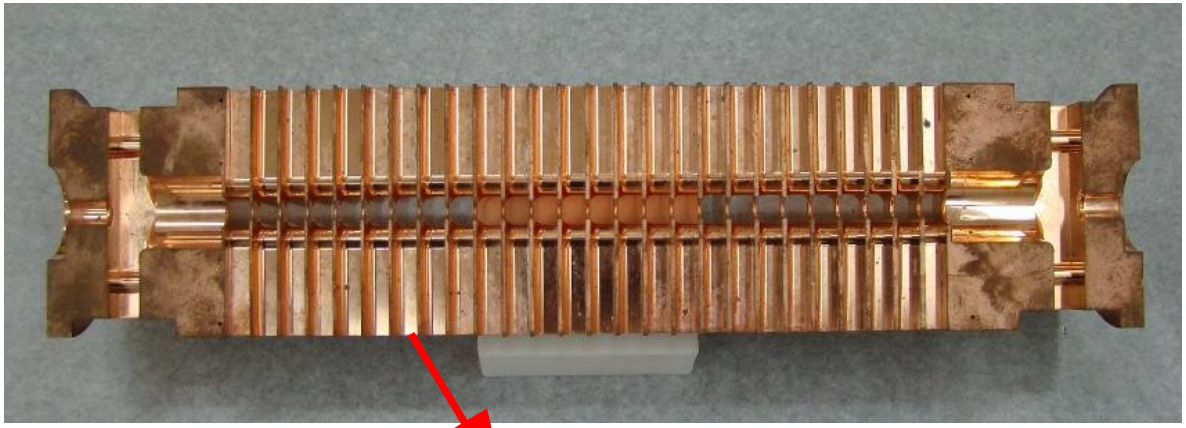


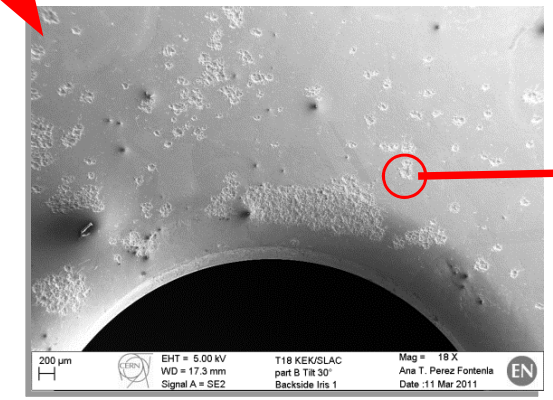
Accelerating structure

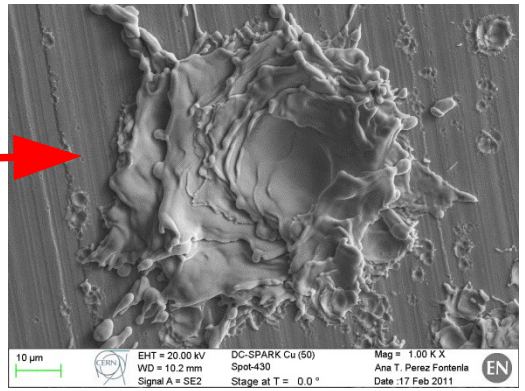


Cross section of a structure

CLIC: plasma & materials physics







Problem: the high fields causes frequent electric arcs (breakdowns):

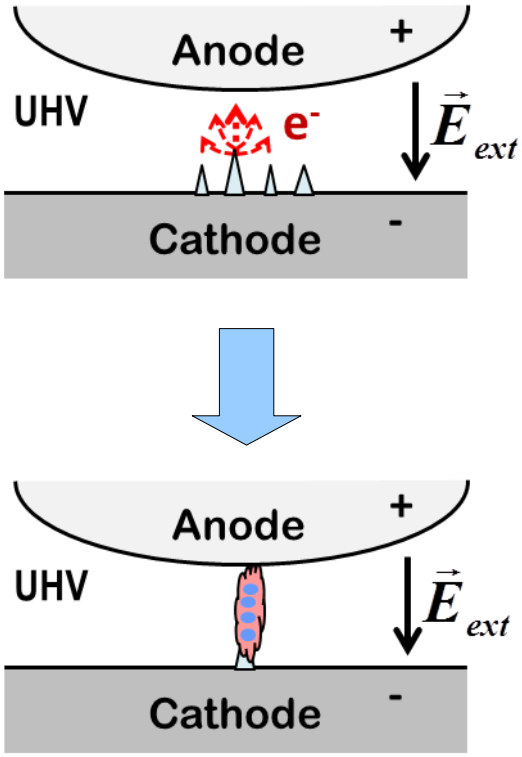
- Lower performance
- Surface damage

Nanotips (cause of the arcs?)

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

But tips are not likely to be seen after vacuum breakdowns

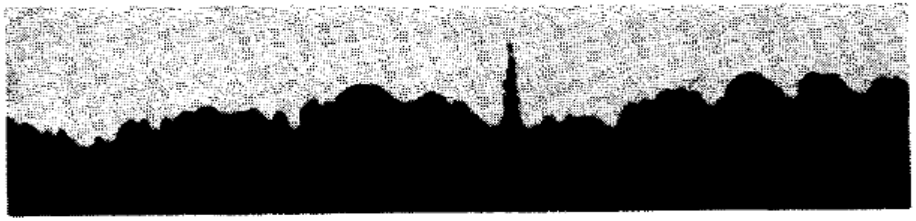
Observations of nanotips with aspect ratios of ~10 are rare, which raises the questions: **How stable are nanotips? How do they form?**



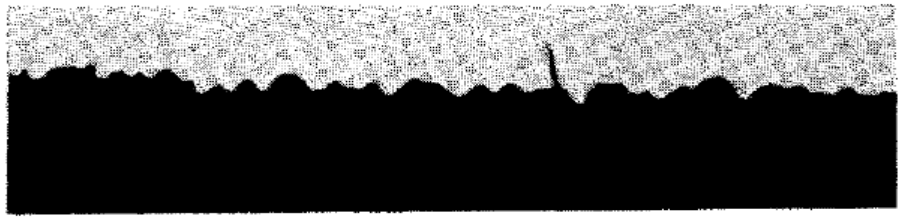
Field-emitting tips appears and a plasma is formed

The plasma burns (breakdown) and the tips are destroyed

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.

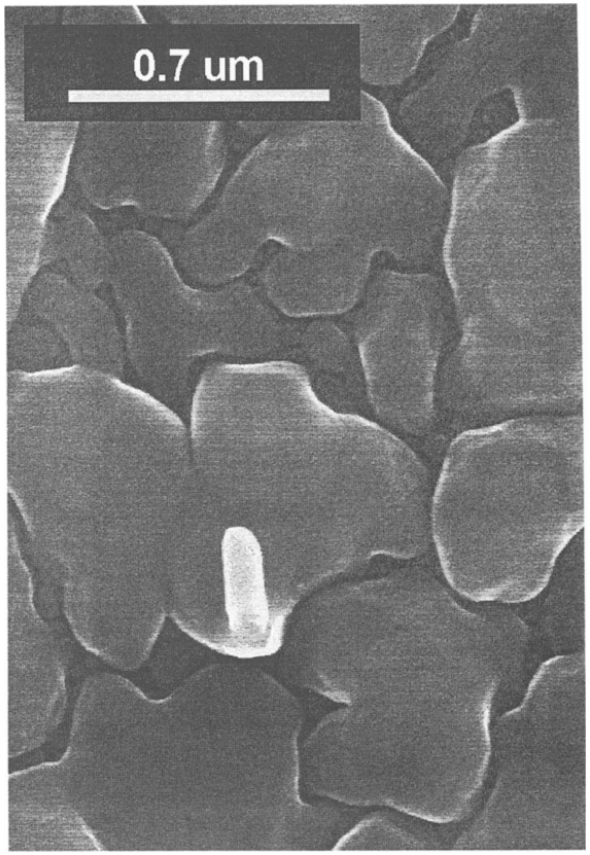
They used a field of 10 MV/m and a 10^{-5} Pa vacuum.

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

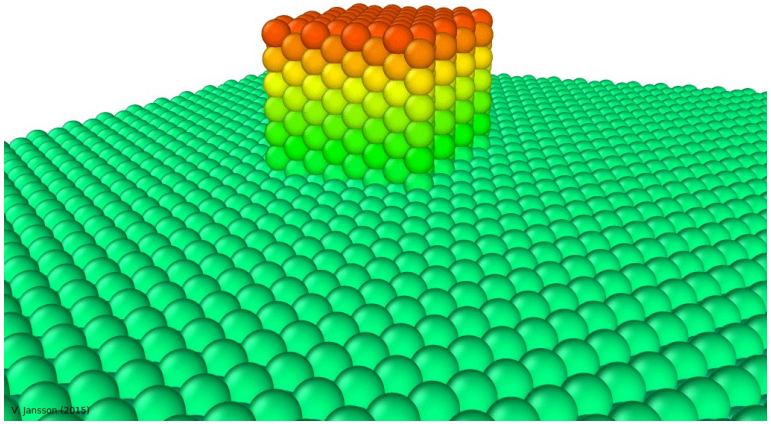
The tip was produced using metal organic chemical vapor deposition of Cu on quartz

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



[F. Atamny, A. Baiker. 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

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

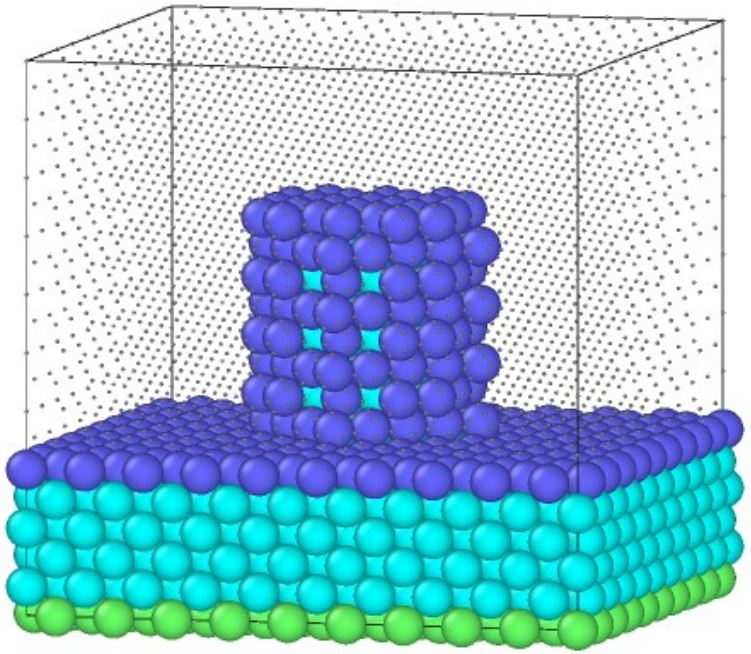
where

  - ν is the attempt frequency
  - 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

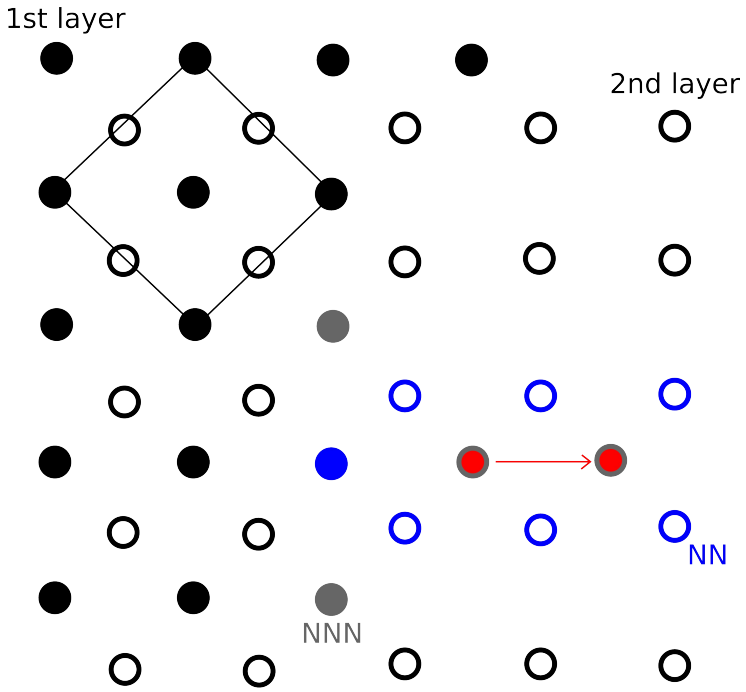
- Designed to simulate the surface evolution on the atomic scale
- Only surface atoms (blue) can migrate by jumping to vacant lattice sites on a rigid 3D lattice
- Bottom atoms (green) are usually fixed
- Different surfaces are possible: (100), (110) and (111), but not different grains
- Only fcc and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



Kimocs

A KMC code for the surface

(100) surface

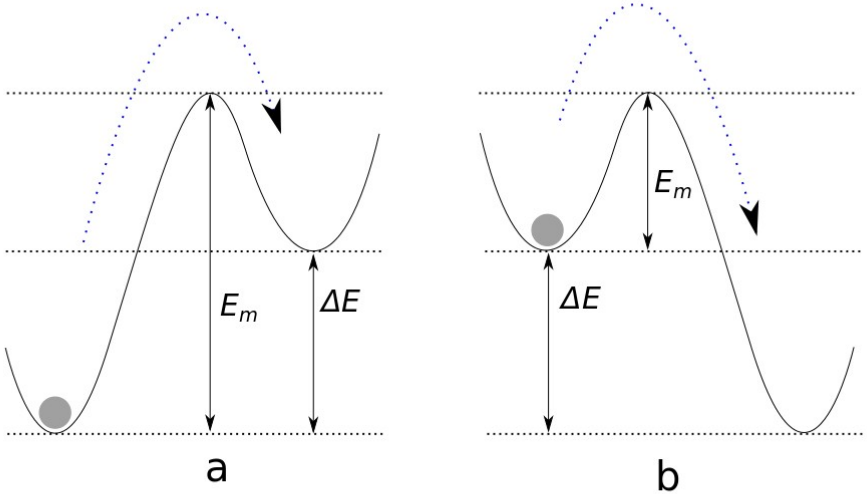


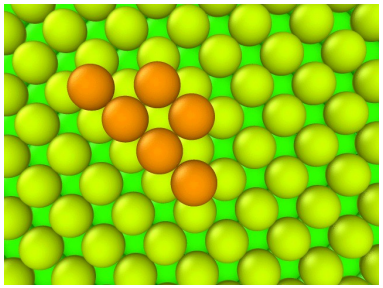
$E_m(5,3,5,1)$

- 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

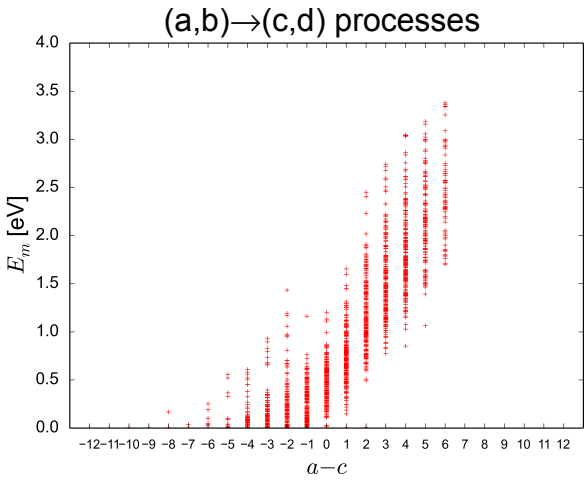
Calculations of the migration energies, E_m





(6,2)→(7,2)

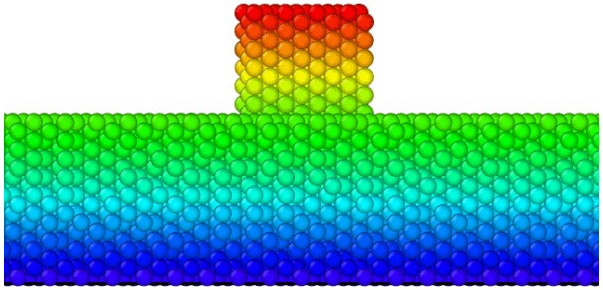
- E_m for a process depends on the local atom configuration and can be described as (1nn,2nn)→(1nn,2nn)
- Thousand of configurations has to be considered
- The Molecular Dynamics method Nudged Elastic Band (NEB) is used



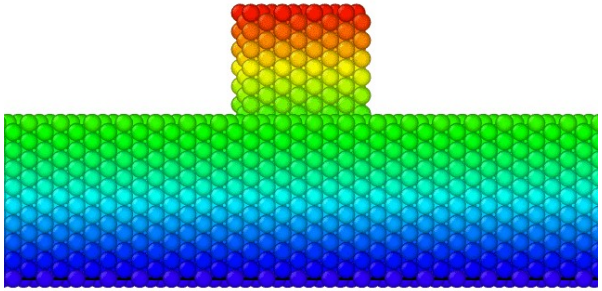
E. Baibuz, V. Jansson

The attempt frequency ν

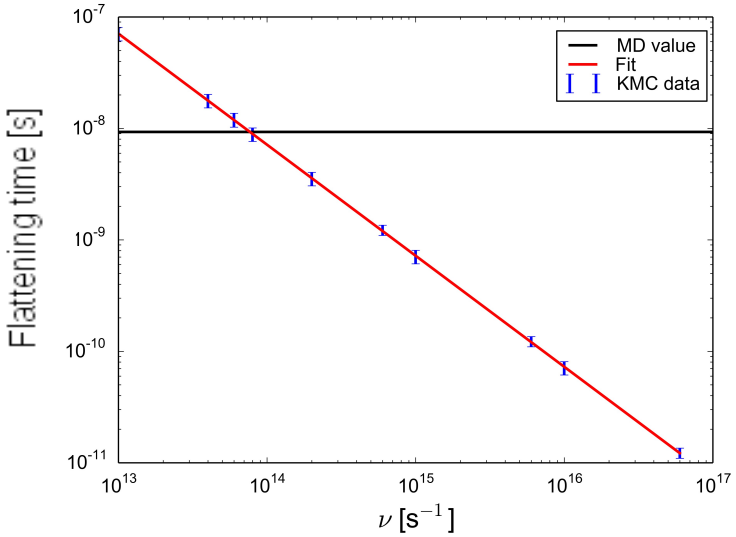
MD



KMC

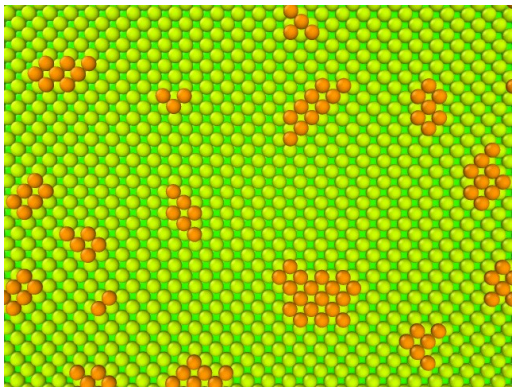


- Since all processes are atom jumps, ν can be considered a constant near to the Debye frequency of Cu, $4.5 \cdot 10^{13}$ s^{-1}
- Our value $\nu = 7 \cdot 10^{13}$ s^{-1} is obtained by fitting to MD simulation results of the Cu tip flattening proces

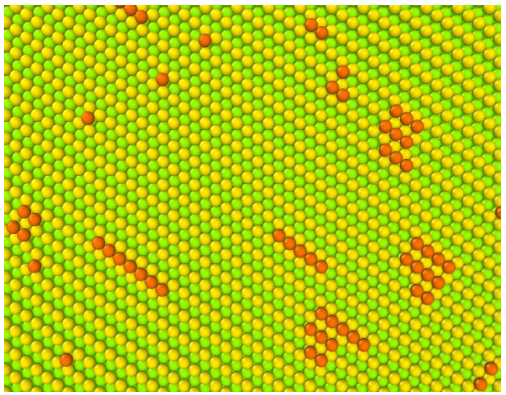


(100), (110) and (111) surfaces

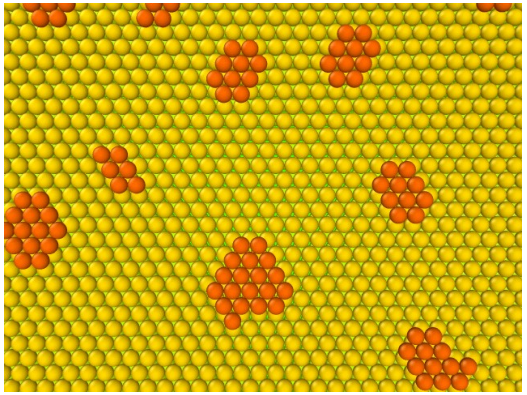
Kimocs simulations: Adatom islands



(100)



(110)



(111)

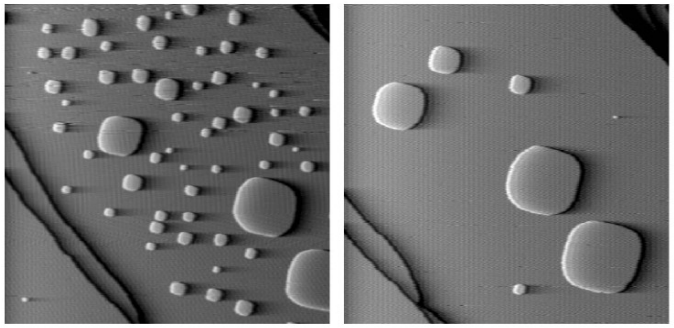
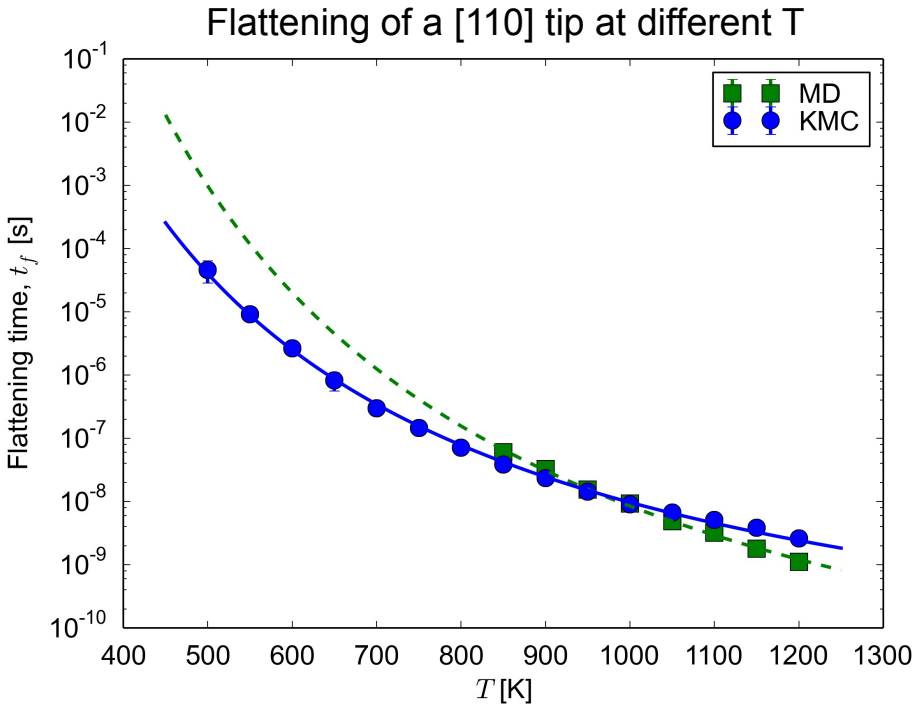
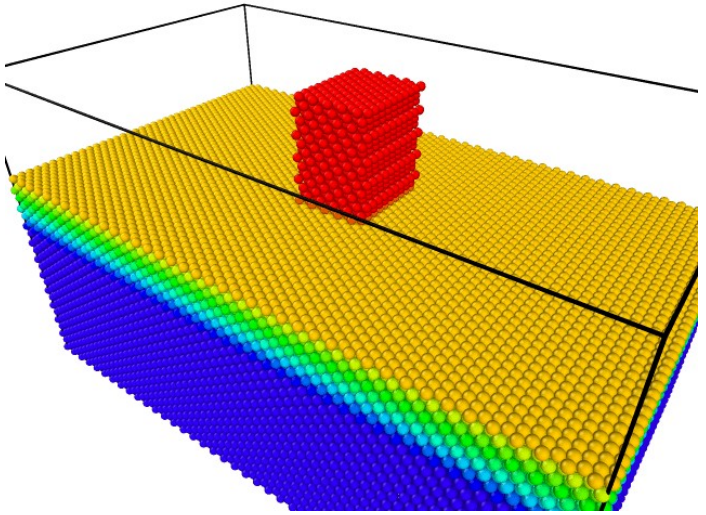


FIG. 2. Two 300 nm × 300 nm STM images, separated in time by 20 000 s, showing island ripening on Cu(001) at 343 K.

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

Tip flattening: KMC vs MD

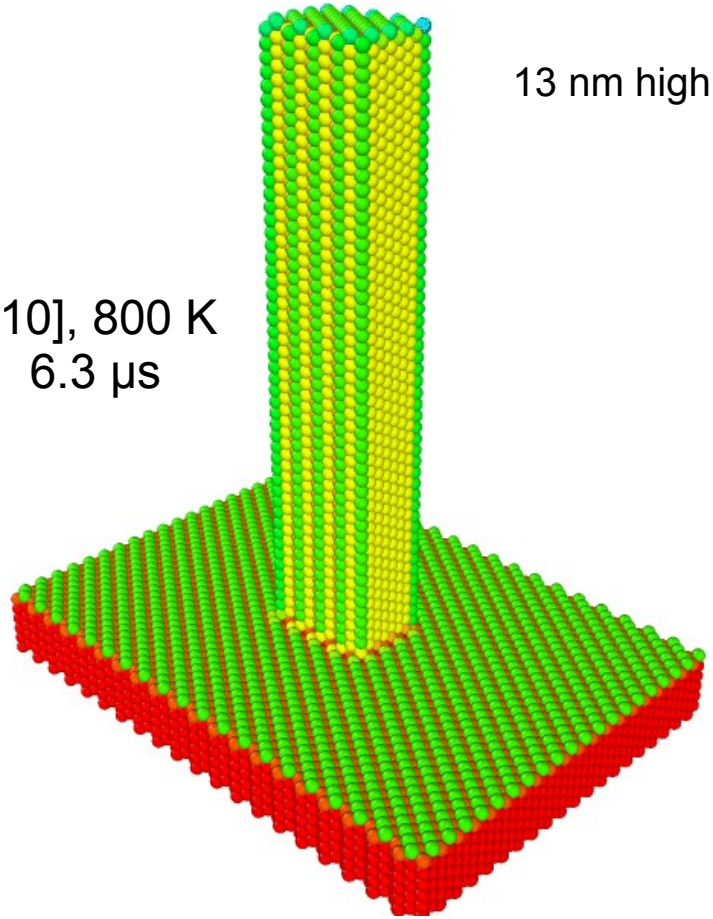




- Good agreement at 850—1150 K
- Strong temperature dependence
- KMC is ~100 times faster than MD

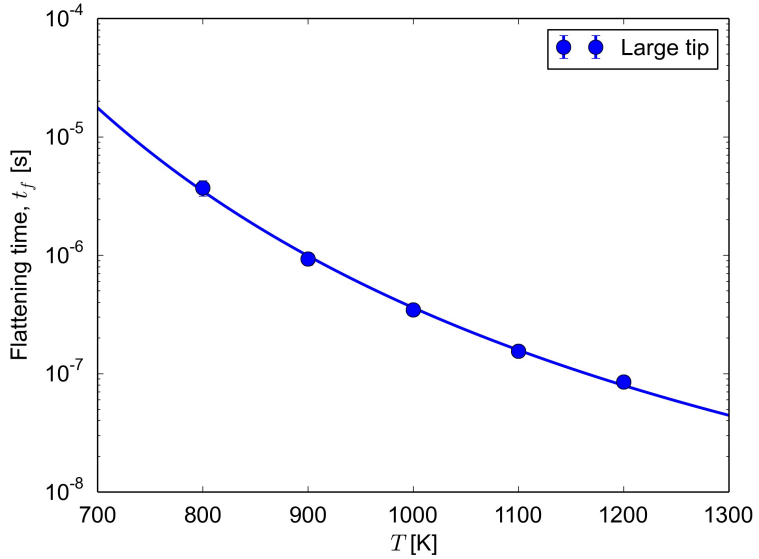
Stability of large tips

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

Summary & conclusions

- Our Kinetic Monte Carlo surface model
  - Allows us to study surface evolutions at ns to ms
  - Works for Cu, Fe and W (Au in progress)
- Cu tips can be stable for hours at room temperature
  - High dependence on the temperature
- Inclusion of the electric field in progress
- Long term goal: understand the arc problem in CLIC

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and
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Cu(100), 5.5 ps, 700 K