MD Simulation of defects in nanocrystalline copper in strong electric fields

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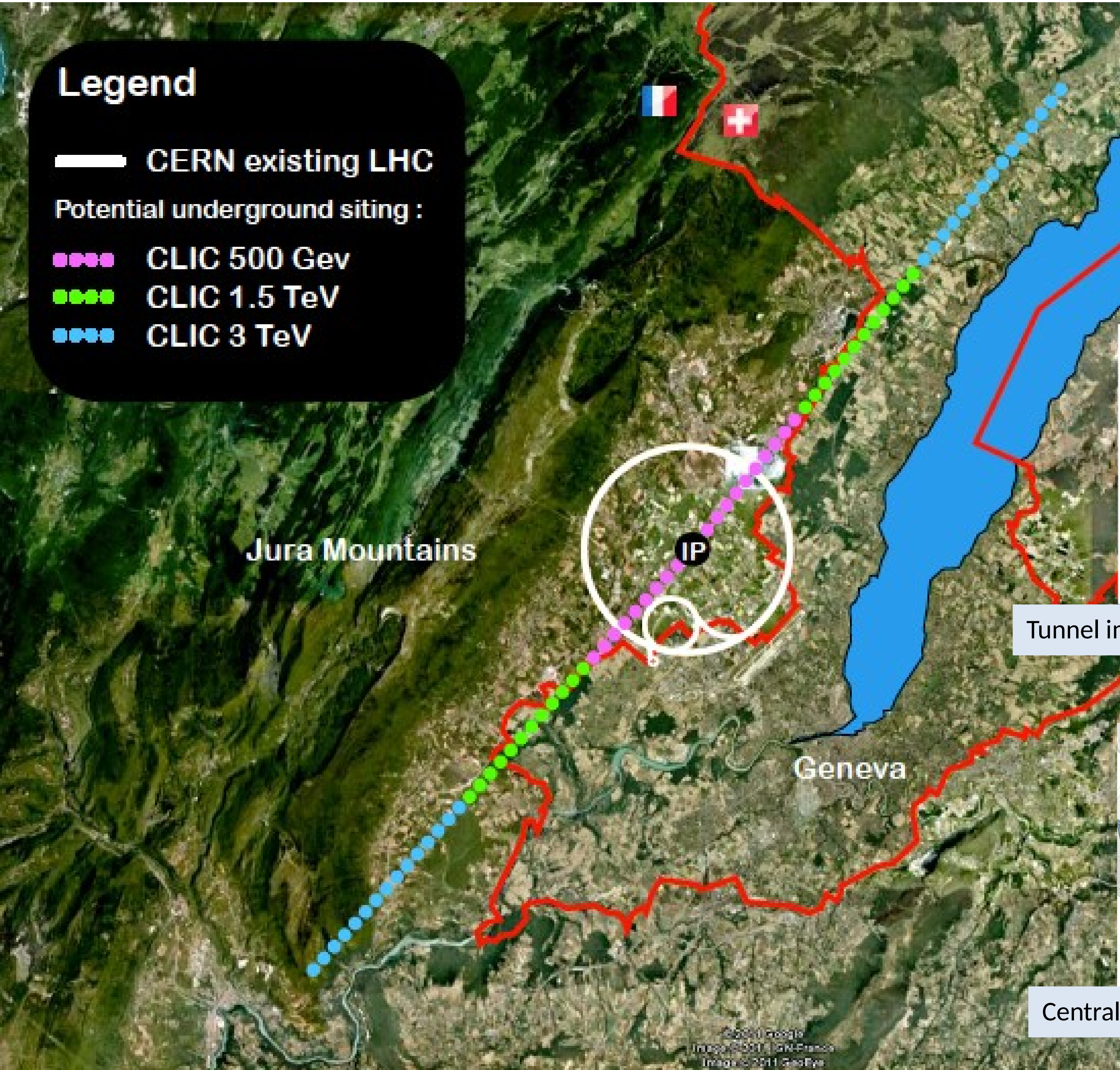
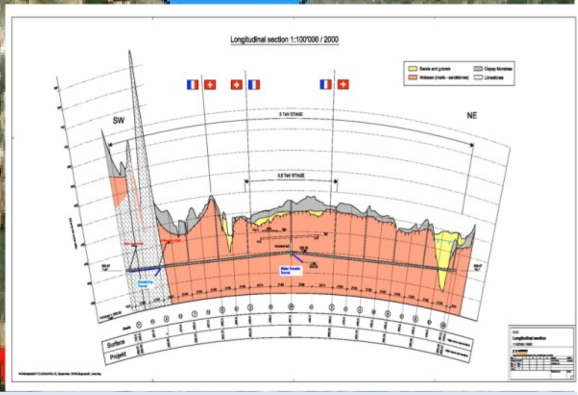
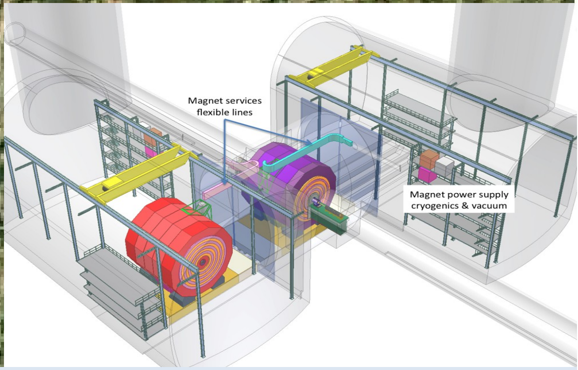
CLIC near CERN





Tunnel implementations (laser straight)



Central MDI & Interaction Region

Some CLIC facts

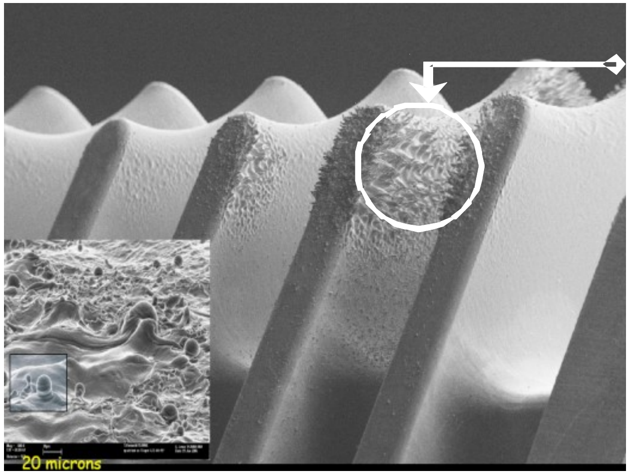
- Accelerator length 50 km
- Accelerating field 100-150MV/m
    - Electrical breakthrough in air at 3MV/m
    - Theoretical electric breakdown in CLIC ~11-12 GV/m
- High elelectric field is needed to minimize the length of the accelerator
    - High electric field leads to repeated electrical breakdown problem
- Electron-positron beam collisions at the energies from 0.5 TeV to 5 TeV

Electrical breakdowns in CLIC

Electrical breakdowns at CLIC accelerator accelerating structure materials

Accelerating el. field 100-150 MV/m

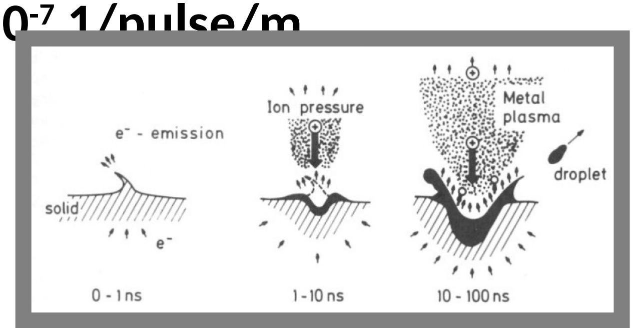
- Accelerating structure damage due to electrical breakdowns
- Might cause the loss of the accelerated beam
- Local field enhancement up to factor 100
- Field enhancement caused by „invisible needles“



Highest RF field gradient

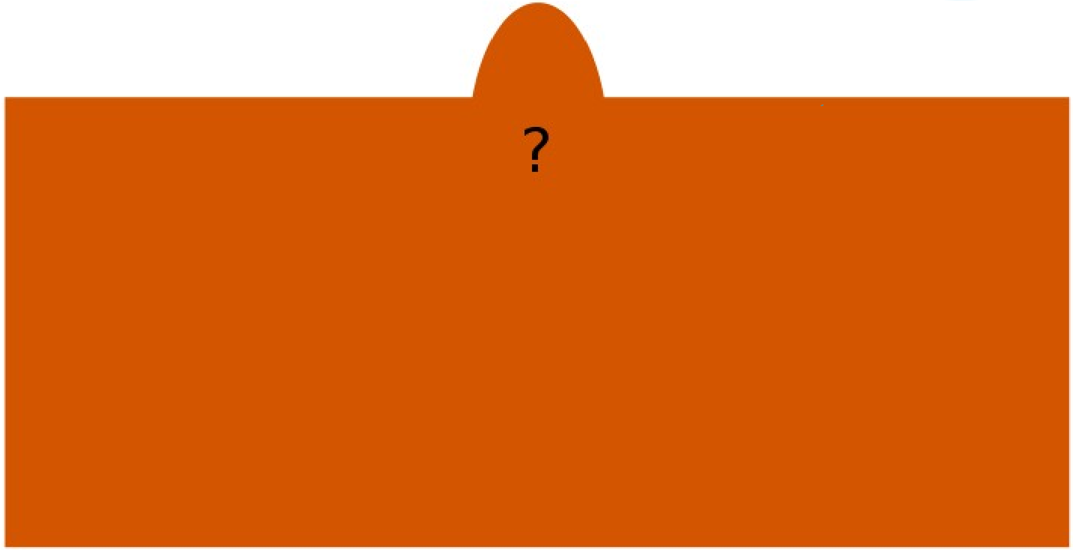
R. Behrisch, Plenum, 1986
B. Jüttner, 1979

Electrical breakdown rate must be decerased under $3\cdot10^{-7}$ 1/pulse/m



Simulating the appearance of the protrusions

- Protrusion growth leads to the increase in the local electric field,which leads to a self-reinforcing process



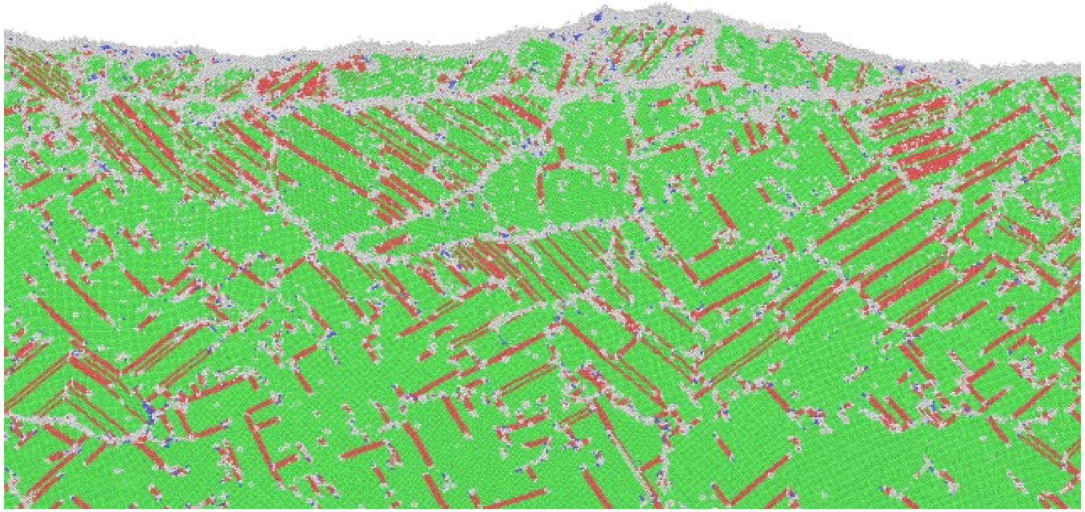
- Material defects as the cause?
  - Pre-existing voids can cause protrusion growth
  - So can impurities in the form of precipitates

- BUT, the onset electric fields still too high

Nanocrystalline copper

- Cu sample obtained from an explosive welding simulation
  - Severe plastic deformations due to the applied stress and temperature
  - Similar treatment and conditions as during a breakdown event
- Initial sample
- Opportunities to study grain boundary effects and influence of rough surfaces

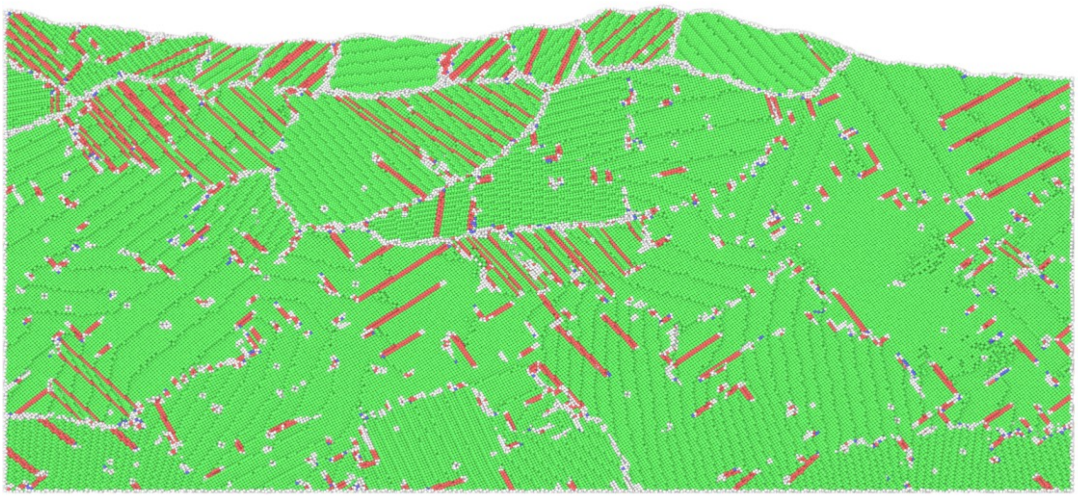
Initial sample



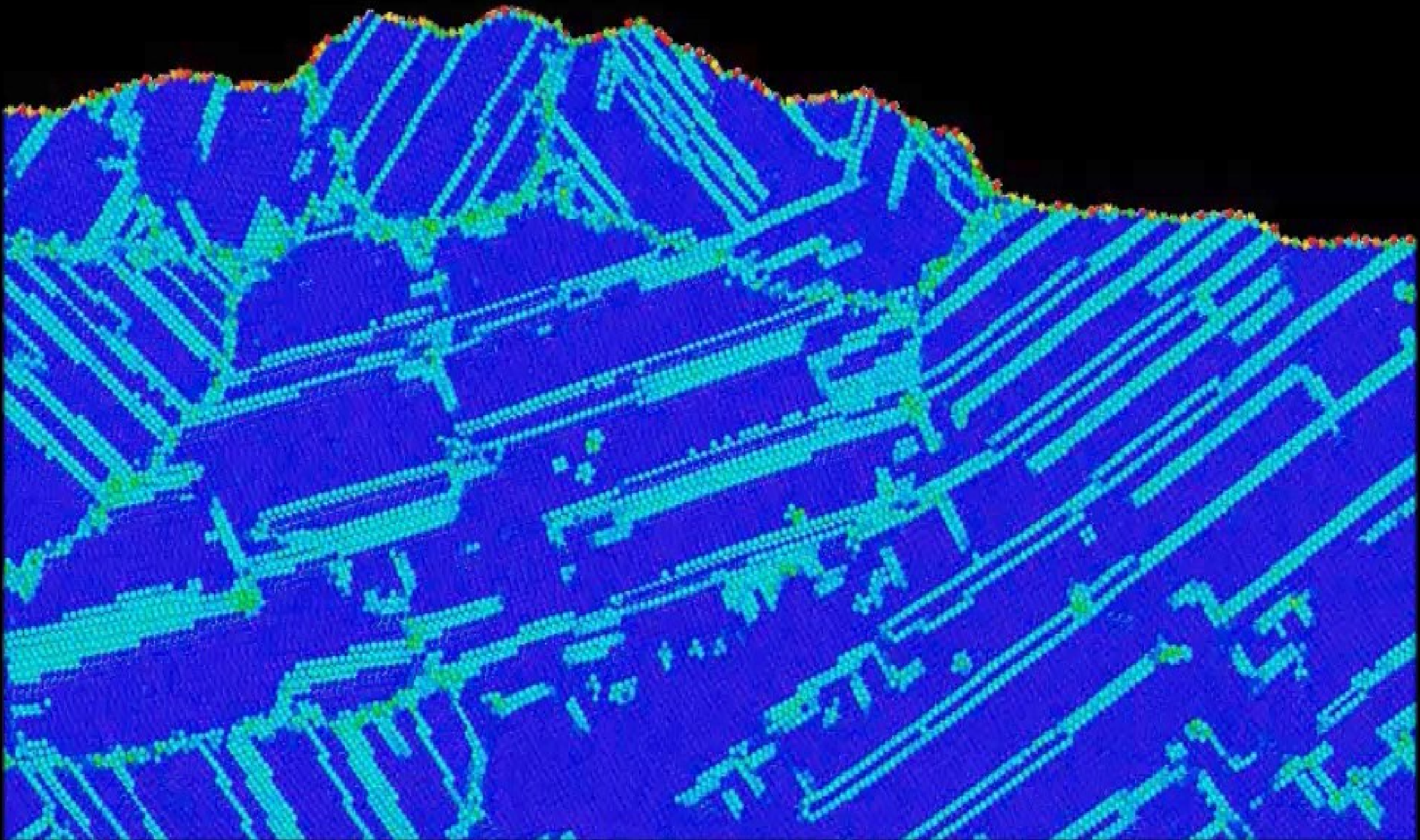
Inside look of the initial sample

Preparing the sample

- Defect reduction methods:
  - Conjugate-Gradient minimization scheme to relax the lattice
  - simulated annealing to 0.8Tm for 200ps to grow the grains and reduce the number of stacking faults
- Velocities for the atoms are created with a random number generator
- Temperature is controlled with a thermostat
- Final sample contains several defect free grains and a number of surface intersecting grain boundaries

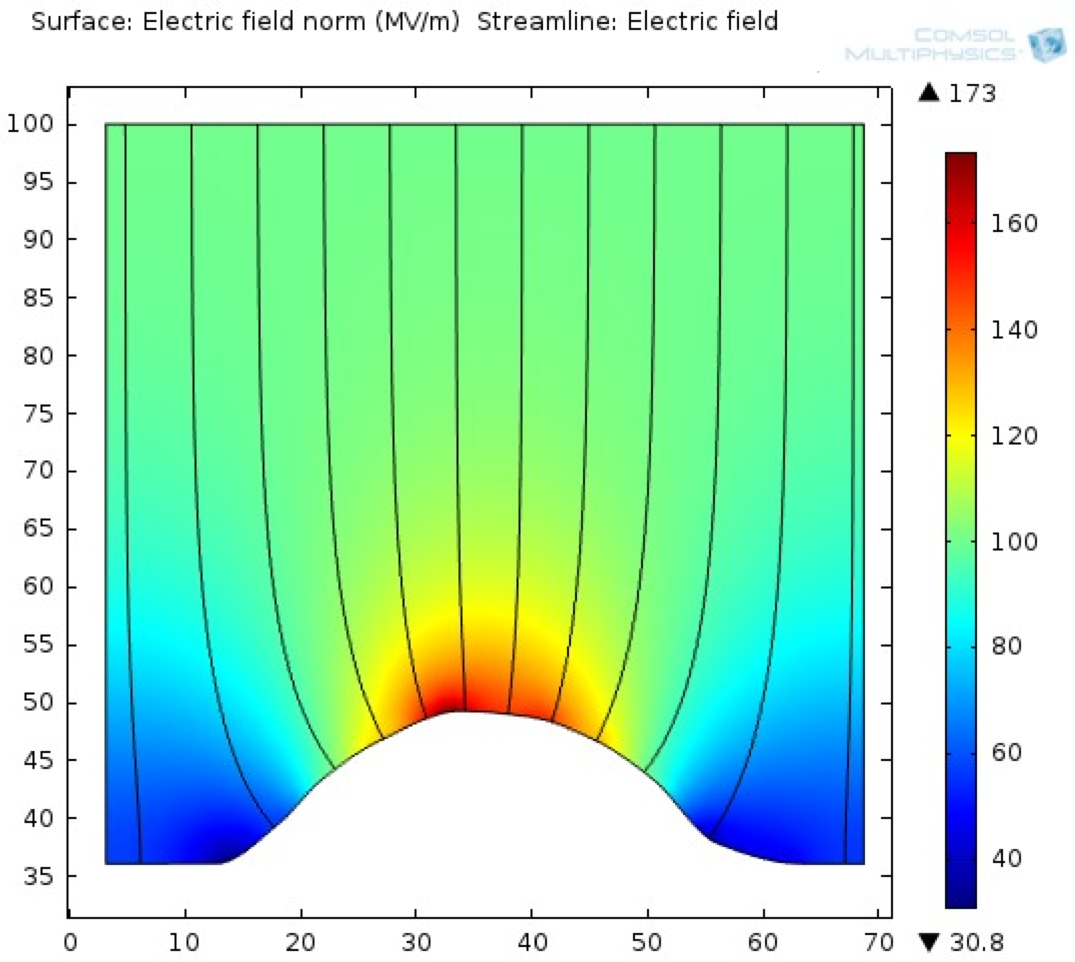


Final optimized and relaxed sample



Coupling Electrodynamics and MD

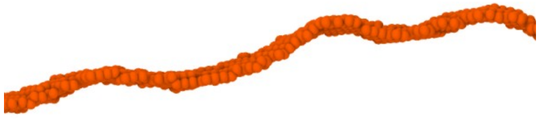
- Imperfect surface leads to nonuniform electric field distribution
- In-turn leads to nonuniform stress distribution, which has to be taken into account
- Charges not explicit in MD
- Have to use multiscale approach
- Finite Element Method for finding the electric field distribution
- Stress on the surface scales with E^2



Atom-to-Continuum problem

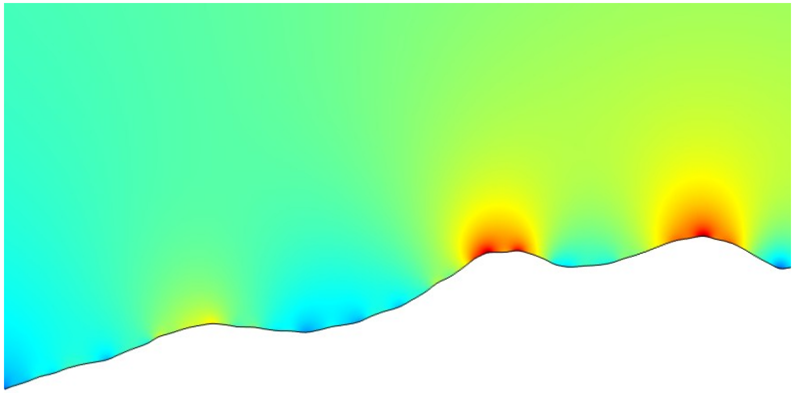
- Surfaces are not well defined in MD
- Algorithm using Coordination analysis to dynamically find the surface atoms during a simulation
- Algorithm for smoothing the position of the atoms to avoid artificially sharp edges
- Importing the surface into COMSOL
- Piece-wise cubic splines to create a smooth, mathematical surface
- Electric field calculations in COMSOL
- Prepared a model to move back from the continuum representation to atomic
- Necessary to average the applied stress distribution

1. Atomistic surface detection using common neighbor analysis:



2. Surface reconstruction through smoothing:

3. Calculating the surface roughness enhanced el. field:



Future work

- Implementing an algorithm for using the el. Field distribution from FEM to apply stress on the surface
- Not trivial, current implementations are not satisfactory
- Dynamically exchanging information between the atomic and continuum representations of the system during a simulation
- Maybe possible to implement in LAMMPS?
- Atom-To-Continuum package in LAMMPS is being developed further at the moment
- Dynamically linking COMSOL with LAMMPS or other MD code?
- DFT/hybrid MD QM code for better simulation of surface charge density?
- Writing my thesis :)

Thank you! Any questions?