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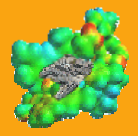

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Atomistic simulations of breakdown triggers: progress report

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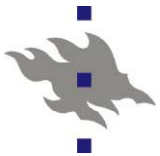

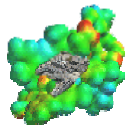

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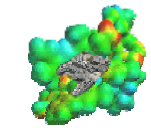
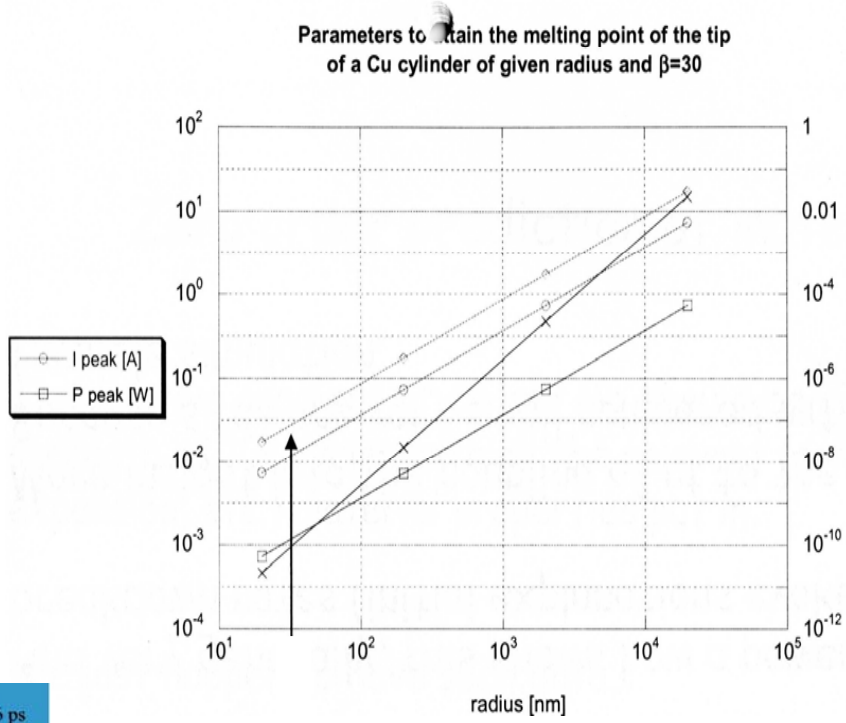
- Our simulation approach
  - Molecular Dynamics + Laplace equation solution
- Results on enhancement factor and atomic charges
- Outlook

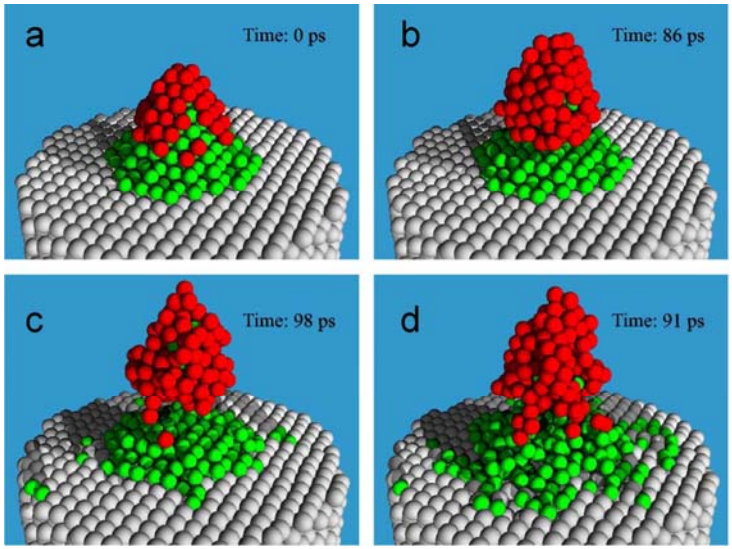
Why atomistic simulation?



Background 1

Sergio Calatroni's results indicate that the breakdown triggers at about 10 nm scale





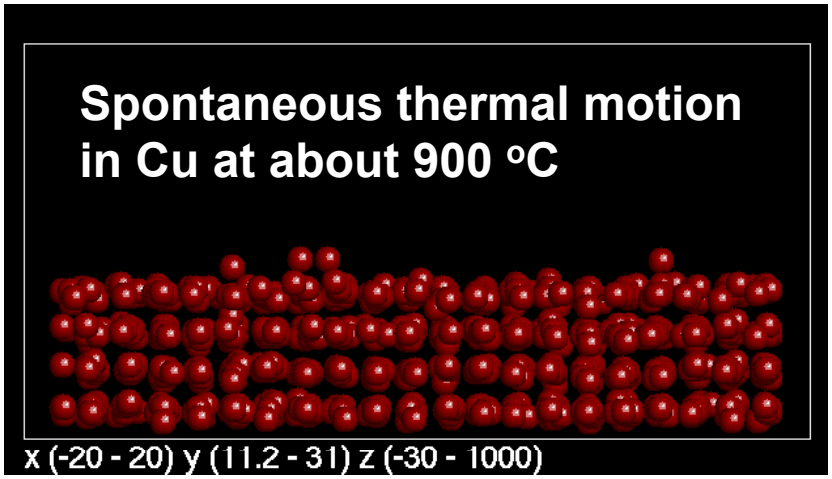
Background 2

Insepov has shown that nanobump + high electric field can lead to the cluster evaporation

[Insepov et al, PRST-AB **7** (2004) 122001]

Motivation

- Breakdown takes place even if the surface is well-smoothed (no rough features are seen in SEM). Also the effect has been observed with many different materials
- => There must be a generic spontaneous roughening mechanism leading to the breakdown
  - But, metal surfaces are known ***not*** to form stable rough surfaces at room temperature
    - Due to thermal motion, some atoms can temporarily become adatoms
  - => Stable roughening requires an electric field!



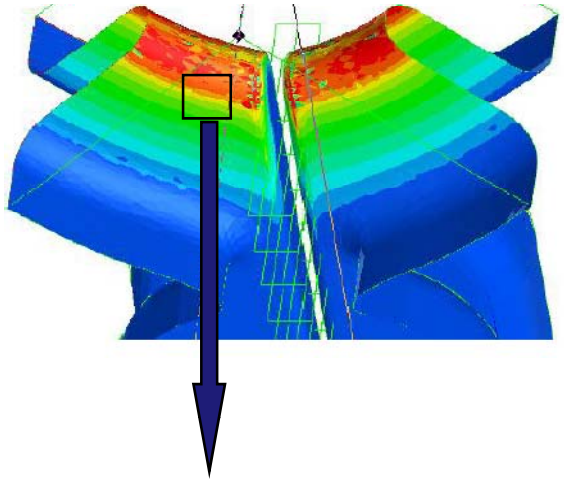
What do we suggest?

Gauss law states

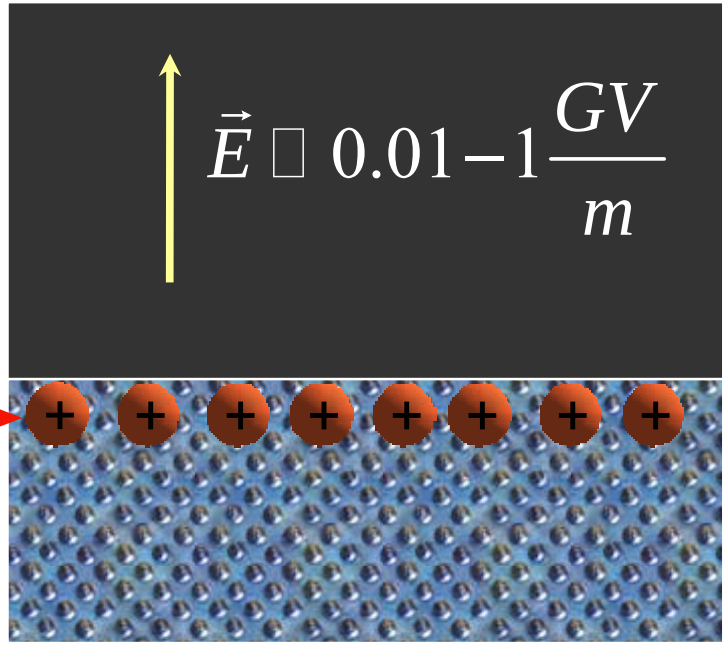
$$\sigma = \frac{Q_{surface}}{A_{surface}} = \varepsilon_0 E$$

Due to the external electric field the surface attains charge

Macroscopic field

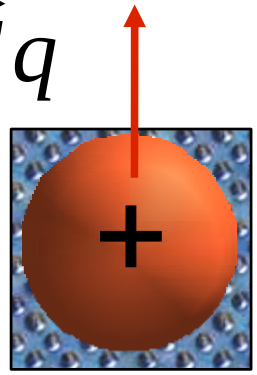


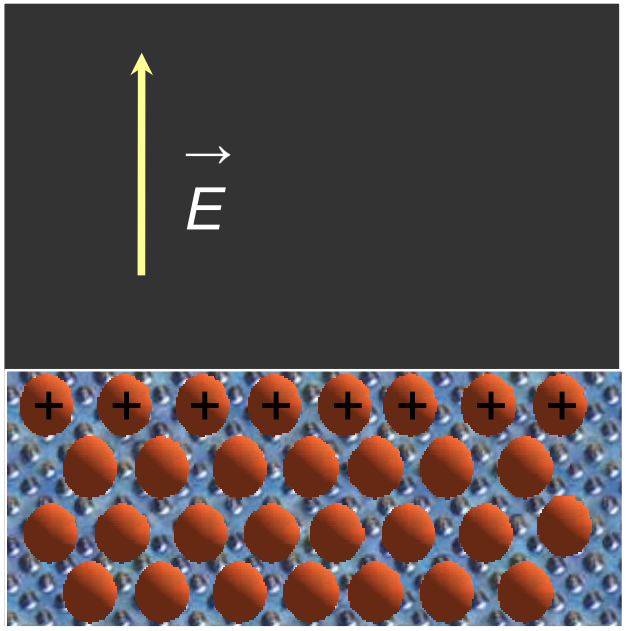
on atomic level:

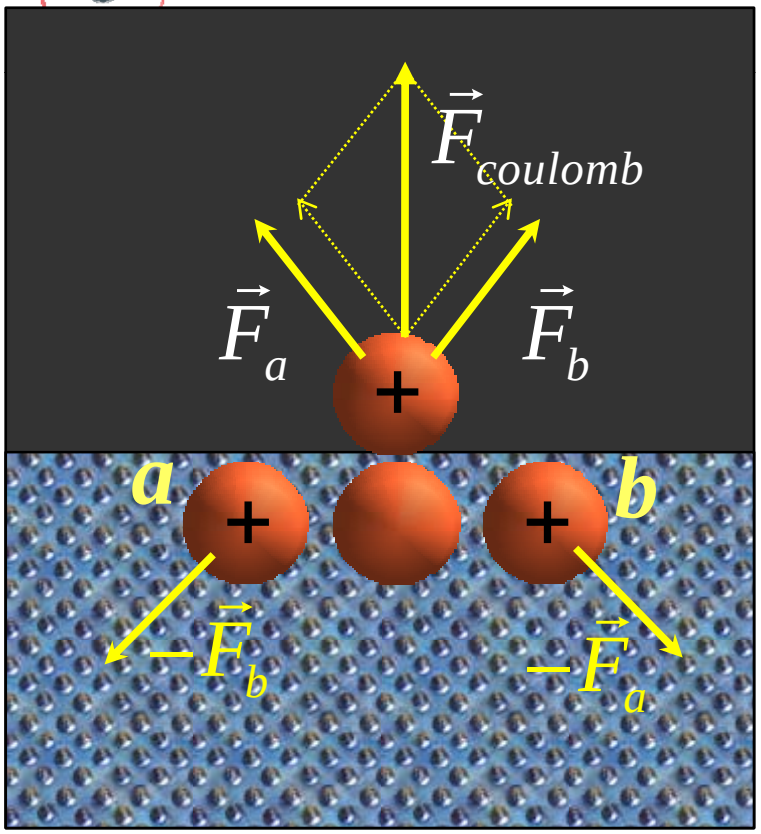


What does this mean for the atoms?

$$\vec{F}_{el} = \vec{E}q$$





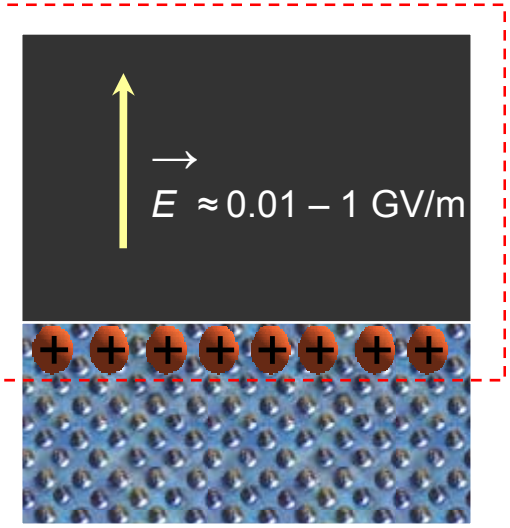


$$\vec{F}_a = \frac{1}{4\pi\varepsilon_0}\sum_i \frac{q_a q_i}{r_{0i}^{\,2}}\hat{r}_{0i}$$

$\vec{F}_{el} + \vec{F}_{coulomb}$ give a driving force for roughening!

Simulation approach

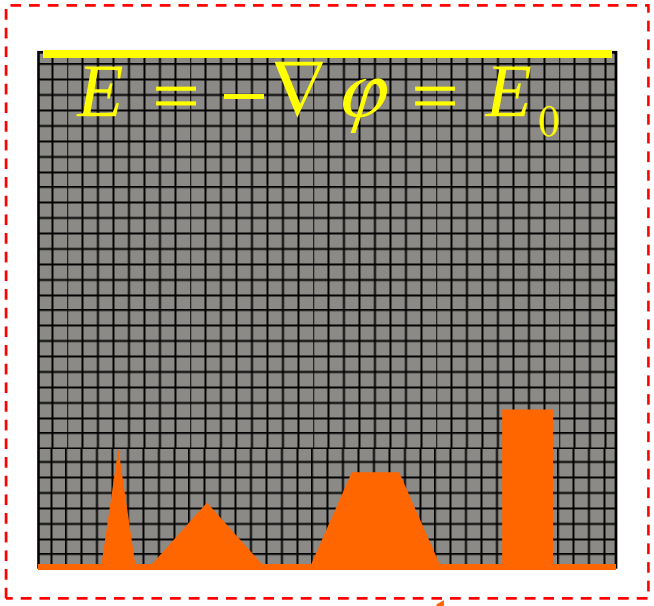
- The current state: we are building a hybrid Electrodynamics/Molecular Dynamics (HED-MD) code to simulate the effect of the electric field



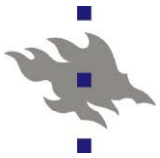
The effect of the electric field is introduced by means of solution of Laplace's equation

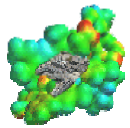
$$\nabla^2 \varphi = 0$$

with the mixed boundary condition



φ=const
(conducting material)





What do we have as output?

- Solution gives $\vec{E}$ at each surface atom $\vec{E}_i$

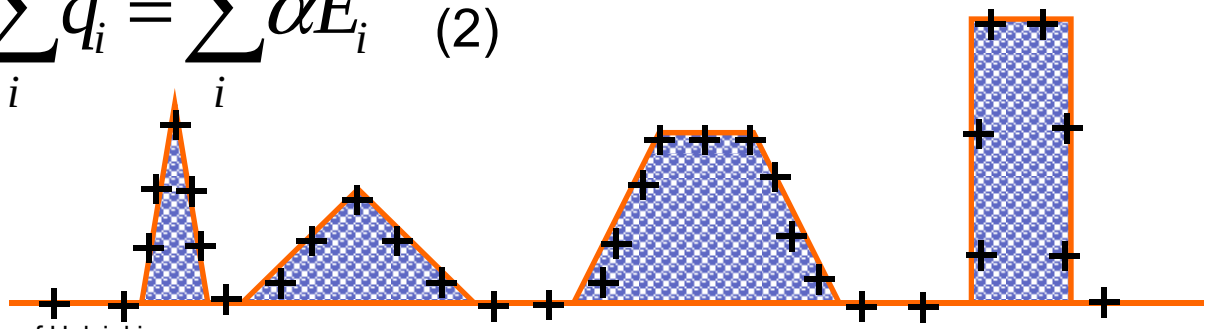
According to Gauss law

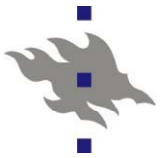
$$Q_{surface} = A_{surface}\varepsilon_0 E_0$$

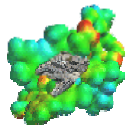
On the other hand, the charge of an atom is proportional to the electric field applied to that atom

$$q_i \propto E_i \Rightarrow q_i = \alpha E_i \qquad (1)$$

$$Q_{surface} = \sum_i q_i = \sum_i \alpha E_i \qquad (2)$$



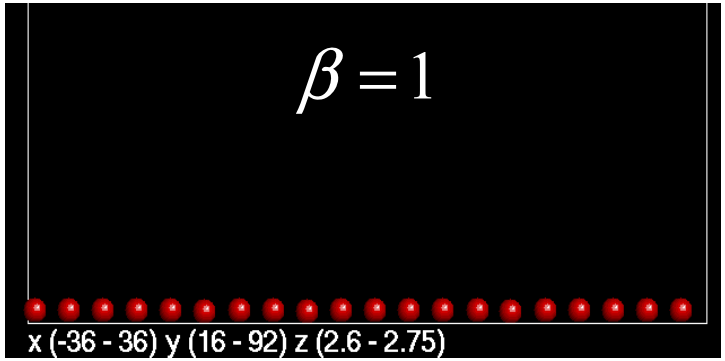


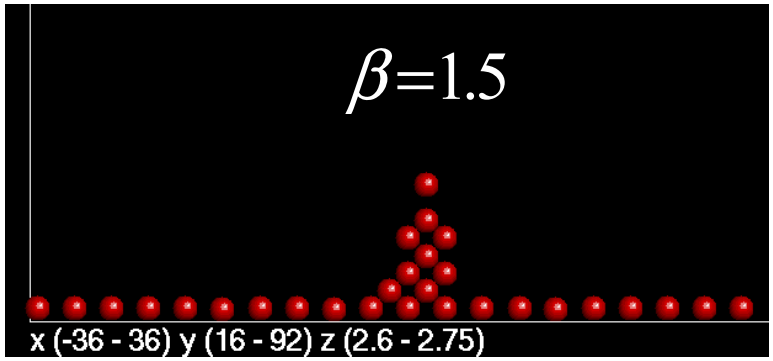


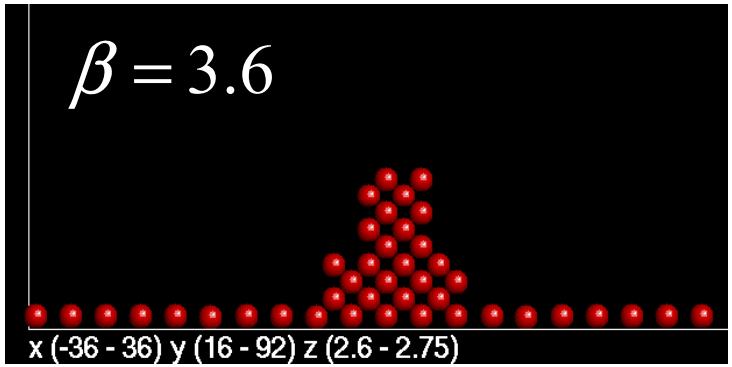
ED + MD: how does this work?

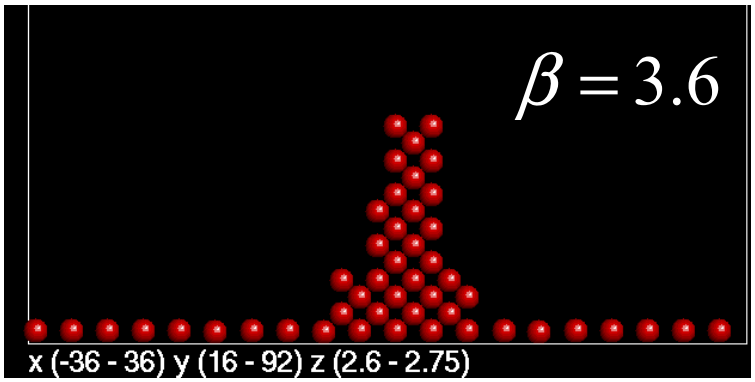
- We embed electrodynamics forces F_{el} and also calculate the Coulombic forces which appear between the charged surface atoms $F_{Coulomb}$, and use the sum of the forces in the MD code to correct the normal atom motions according to the applied electrical field.

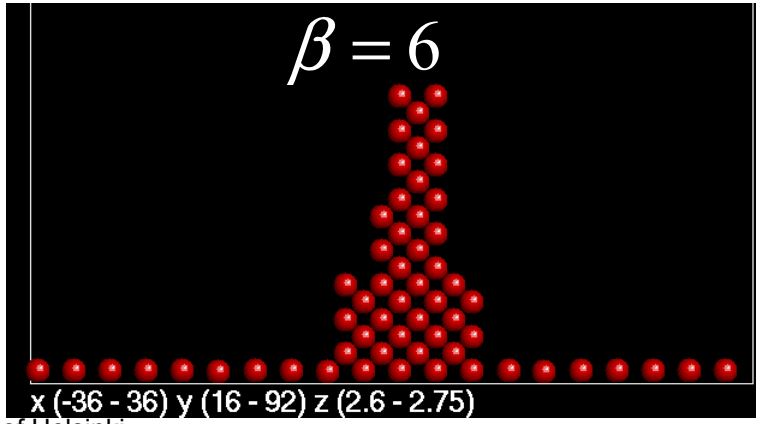
Enhancement factor β for different hillocks on the top of a Cu surface



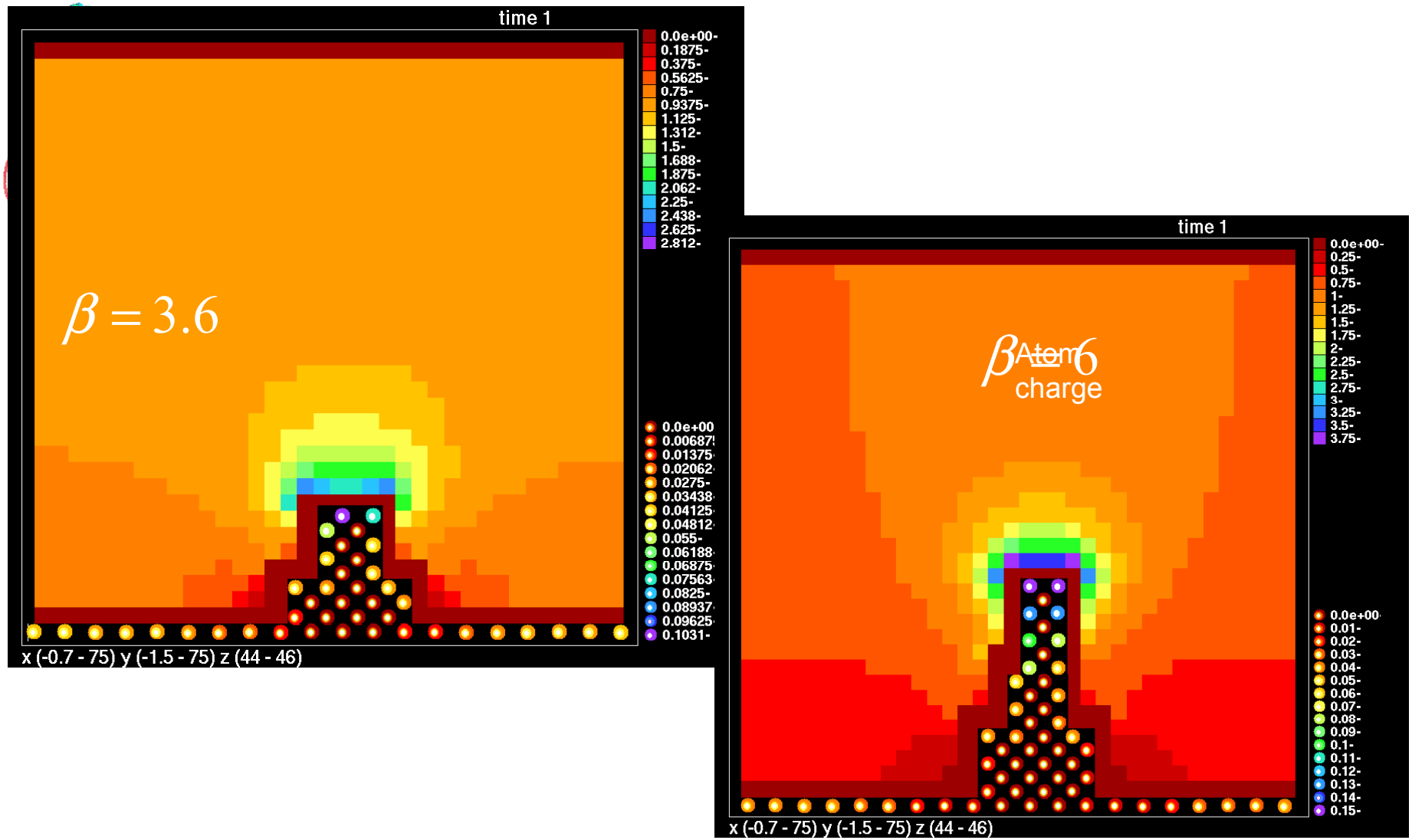


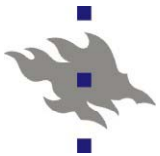


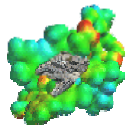




Solution of Laplace's equation for of β=3.6 and β=6 and the charge distribution on the surface atoms







Outlook

- The solution of Laplace's equation must be speeded up due to the huge computational time consumption. We believe this is possible with application of some multigrid scheme
  - we are open for recommendations of suitable efficient methods…
- Dynamic simulation will be the next step to examine the roughening mechanism of the surface