GRK 1161
Disperse Systems for Electronic Applications

Institute for Multiscale Simulation
MSS

Simulation of drying processes in nanoparticulate layers

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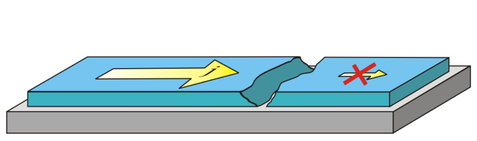
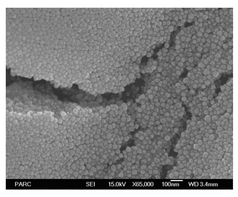
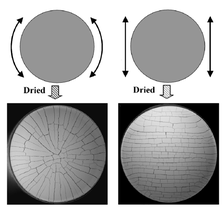
Motivation

The electrical properties of nanoparticulate layers are significantly affected by the drying process of suspensions.
The fast desiccation required by the fabrication processinduces the formation of cracks like in mud or clay [1].





Recent experiments [2] on drying paste show that it is possible to control the morphology of the anisotropic crack patterns that appear during the drying process.



[1] J. Greer, R. Street, J. Appl. Phys. 101, 103529 (2007)
[2] A. Nakahara, Y. Matsuo, J. Stat. Mech. (2006) P07016

Goals

Simulate the cracking mechanism

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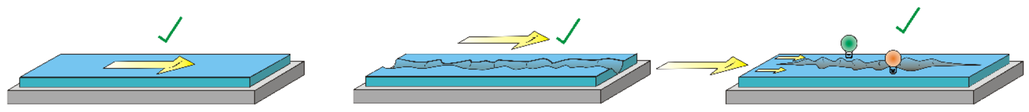
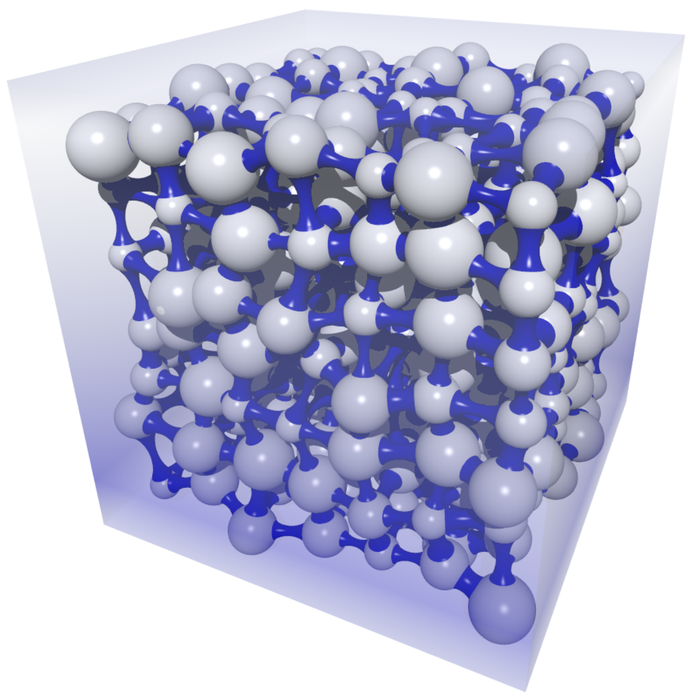
develop methods to

- prevent crack formation
- control crack formation
- utilize cracks



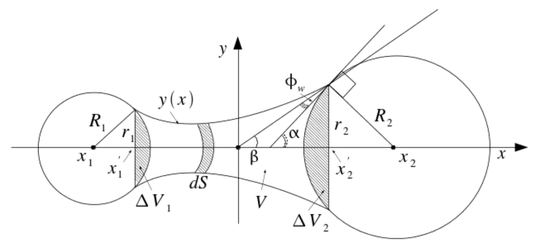
Model



A schematic representation of a multi-phase many-particle system of an almost dry suspension of nanoparticles

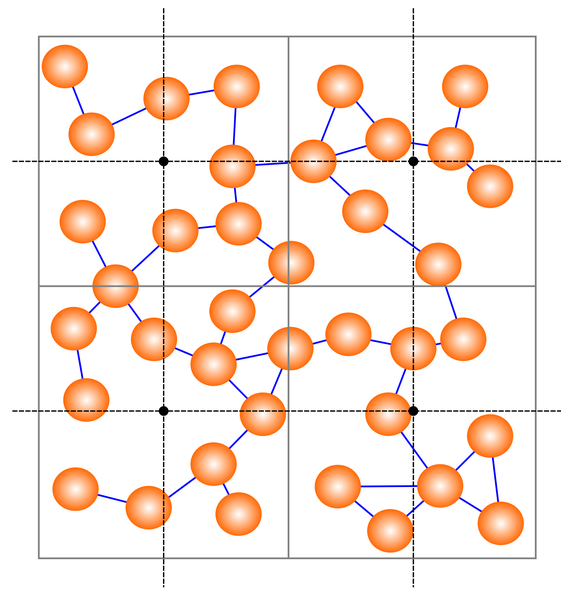
Nanoparticles

- Classical (force based) Molecular Dynamics
- Dynamics of the particles are described by Hertz theory and Newton's equation of motion



Liquid bridges

- The remaining fluid in the system results in capillary forces acting on the particles
- The shape of a liquid bridge is obtained by minimizing its surface under the preconditions that the volume of the bridge and the wetting angle are equal to the desired values.

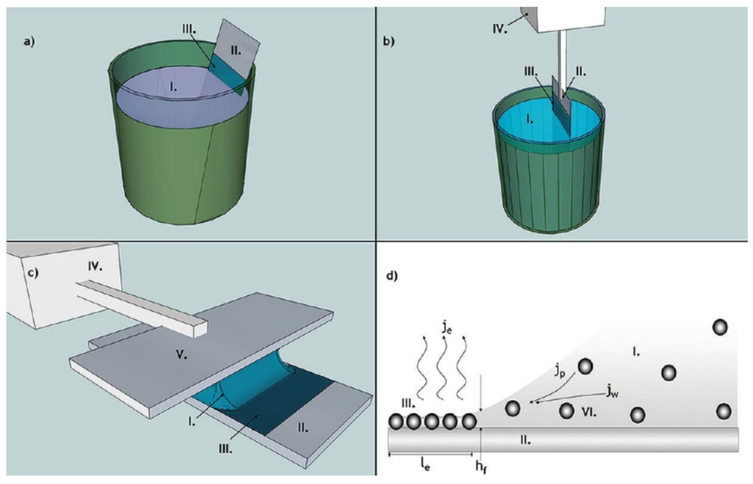


Vapour field

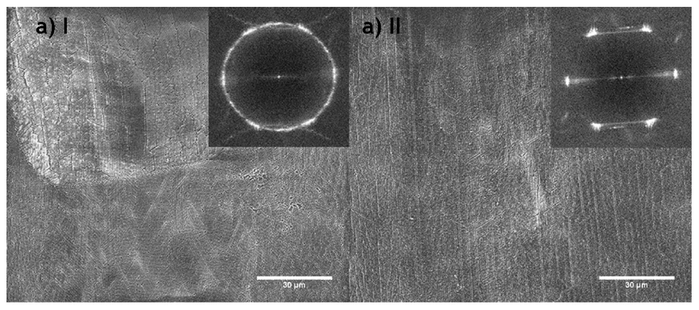
- The simulation domain is subdivided into regular cells with corresponding grid points containing information about partial pressure, vapour concentration and evaporation rate for the respective cell
- A Finite Difference scheme solves the diffusion equation at each grid point

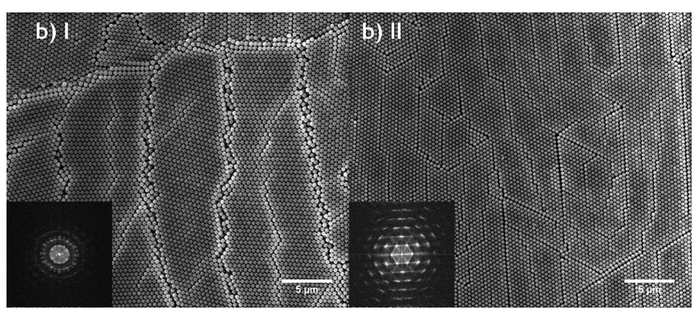
Simulation & Experiment

Convective assembly of 500nm polystyrene particles [3]

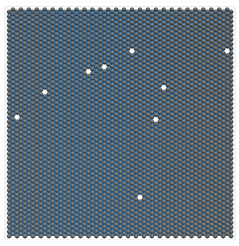


[3] P. Born, S.Blum, A. Munoz, T. Kraus, Langmuir, 27 (2011), 8621-8633.

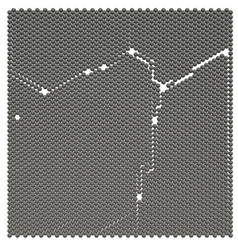




initial configuration



final configuration

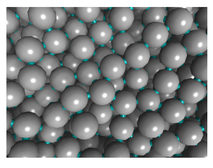


desiccation

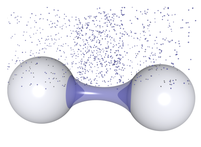
I: large inhomogeneties (holes, double layers, etc.)
II: perfectly crystalline with microscopic voids and drying cracks

Status

Model description of nanoparticles completed



Description of a liquid bridge force model completed



Capable of simulating the evaporation using the Finite Difference Method

Next Steps

- Parallelization and optimization of the code (coop. G. Wellein RRZE, KONWIHR)
- Simulate larger systems of particles
- Further comparison with experimental data

ENGINEERING OF ADVANCED MATERIALS

FRIEDRICH-ALEXANDER UNIVERSITÄT ERLANGEN-NÜRNBERG
TECHNISCHE FAKULTÄT