Crack formation induced by desiccation in nanoparticulate layers

GRK 1161 – TP 8

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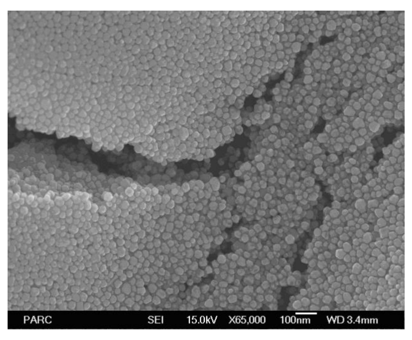
ENGINEERING OF ADVANCED MATERIALS

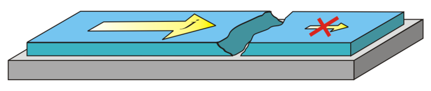
MSS

Introduction

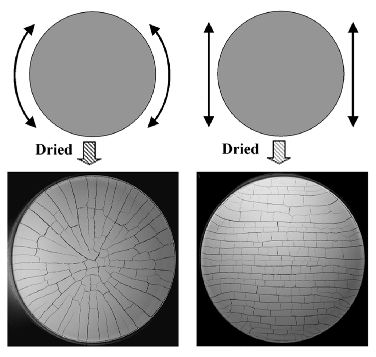
Motivation

The electrical properties of nanoparticulate layers are significantly affected by the drying process of suspensions. The fast desiccation required by the fabrication process induces the formation of cracks like in mud or clay [1]. The formed fractures destroy the conductivity of the nanoparticulate layers. Therefore, this cracking should be avoided by using an optimal drying process.





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.



Objectives

- Study the process of desiccation cracking and its dependency on the physical properties of the suspensions and on the printing process
- Elaborate methods to avoid cracking using optimal process management

Simulate the cracking mechanism

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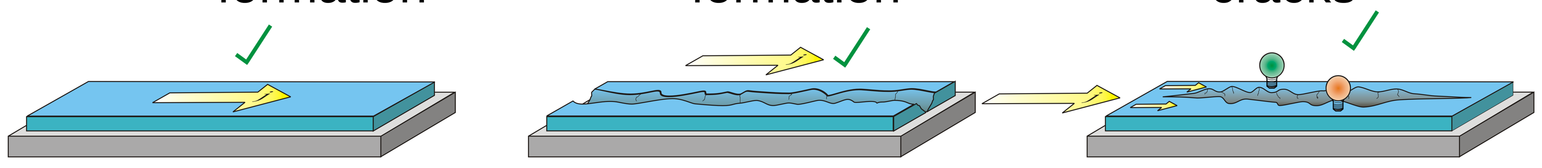
develop methods to

prevent crack formation ✓ | control crack formation ✓ | utilize cracks ✓



Approaches

Model

Vapour Field

$$\frac{\partial c(\vec{r},t)}{\partial t} = \nabla\left(D_c \nabla c(\vec{r},t)\right) + \sum_i q_i^c \delta(\vec{r}-\vec{r}_i)\, Q_i^c(t)$$

Sinks: condensation of vapour
Sources: evaporation of liquid

$Q_i^c = [kg\, m^{-3} s^{-1}]$

Temperature Field

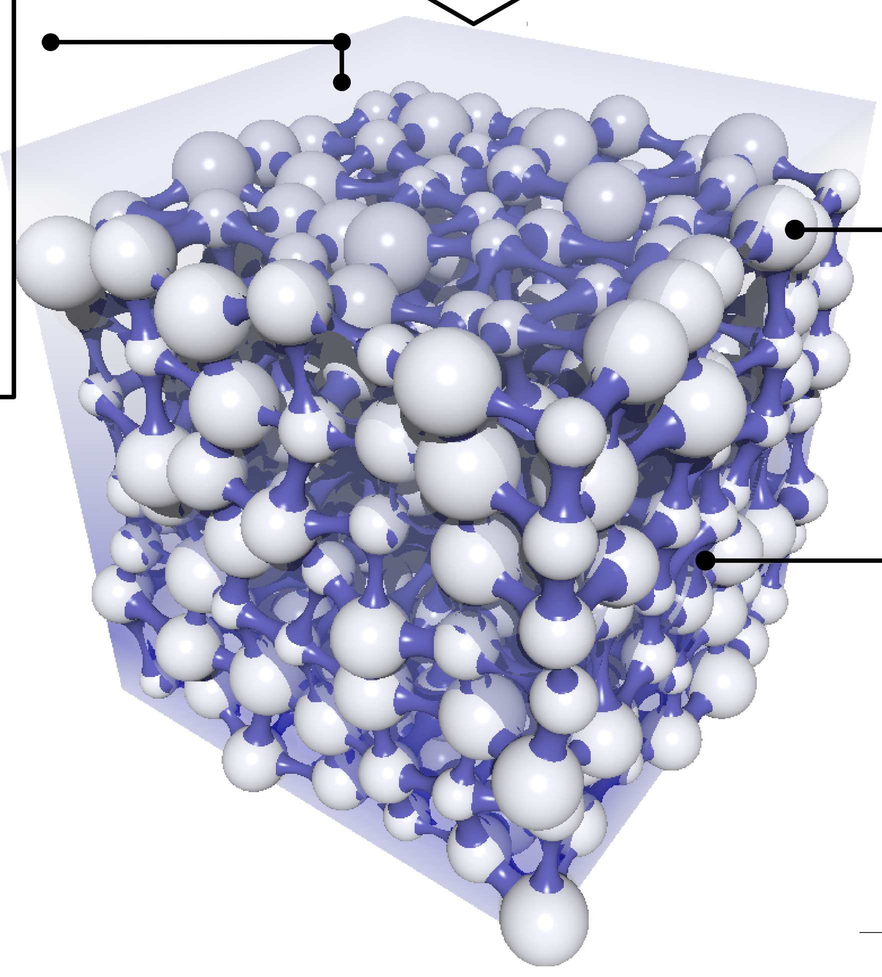
$$\frac{\partial T(\vec{r},t)}{\partial t} = \nabla\left(D_T \nabla T(\vec{r},t)\right) + \sum_i q_i^T \delta(\vec{r}-\vec{r}_i)\, Q_i^T(t)$$

Sinks: evaporation of liquid
Sources: condensation of vapour

$Q_i^T = [J\, m^{-3} s^{-1}]$

$$Q_i^T(t) \propto -\, Q_i^c(t)$$

Multi-Phase Many-Particle System

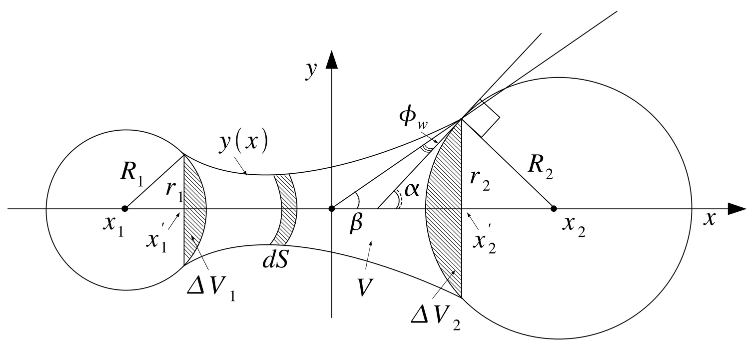


Nanoparticles (ZnO)

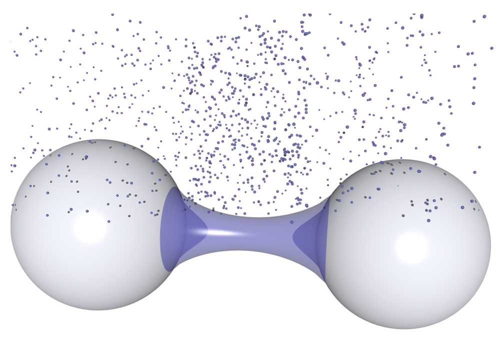
The initial suspension is generated such that its statistical properties agree with experiments.

Liquid bridges

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 ϕ_w are equal to the desired values.



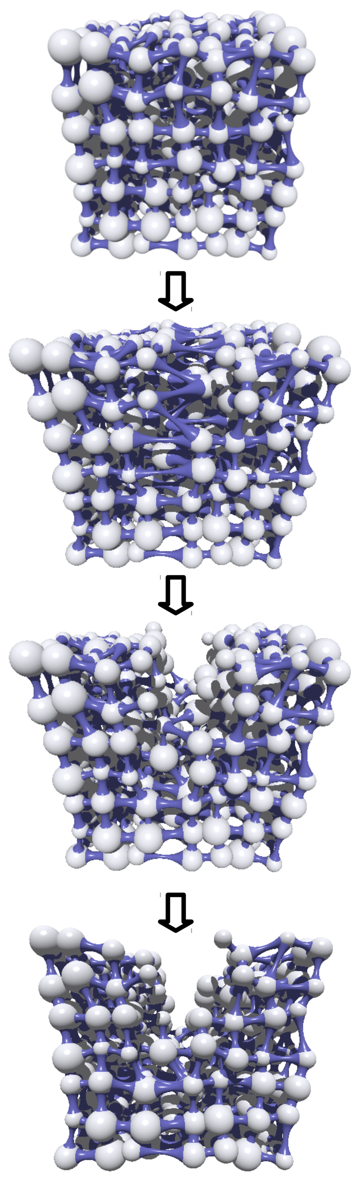
Cracks



The evaporation rate is proportional to the surface of the bridge and depends on its temperature:

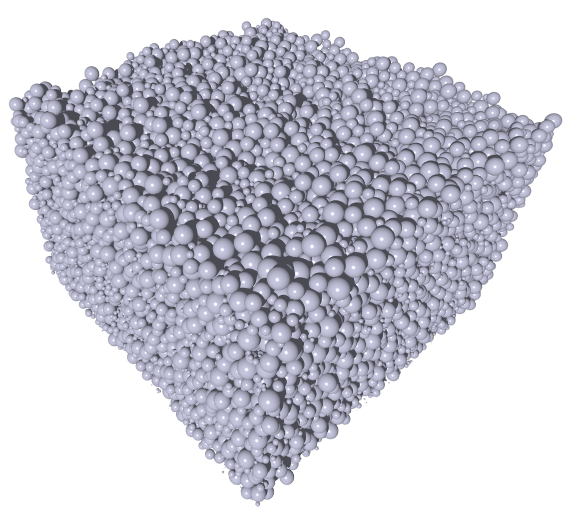
$$Q_i^c(t) \propto -\, S_i(t) f_i(T)$$

Due to evaporation the shape of the liquid bridge changes. As a consequence the interaction forces are altered, which finally leads to the microscopic motion of particles and, thus, to crack formation.



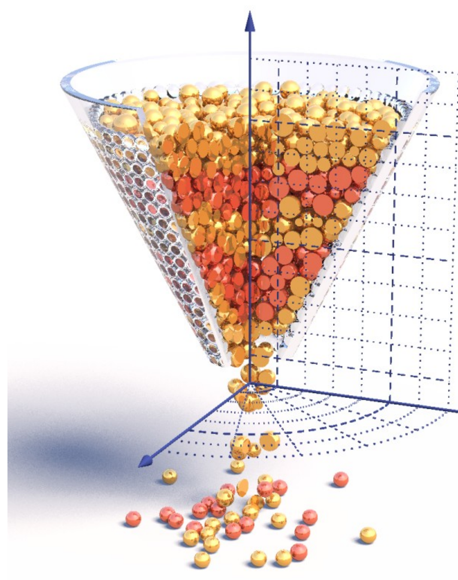
Applied methods

Simulation technique



Method: BTR [5]

Modelling challenges:	Numerical methods and algorithms:
initial structure: nearly dried suspension	modified bottom-to-top reconstruction in agreement with experimental data
evaporation	Monte-Carlo algorithm
steam and temperature field	FEM or Monte-Carlo method
motion of the nanoparticles	classical (force based) Molecular Dynamics



Method: MD [6]

Routing

Working plan

- generate initial conditions according to experimental findings
- specify sources and sinks for the diffusion problems in accordance with the liquid bridge geometry
- implement efficient solution of the diffusion problem with complicated boundary conditions
- derive the forces to be used in Molecular Dynamics
- obtain the criterion for the breaking of liquid bridge
- investigate in detail the prevention, control and utilization of cracks

Collaboration

Internal cooperations:
- TP Roosen: nanoparticle printing technology
- TP Peukert: layer formation mechanisms, measurement of drying kinetics

External cooperations:
- D. Wolf (Theoretical Physics, Duisburg-Essen University, Germany): structure characteristic of nanoparticulate sediments
- A. Formella (Applied Informatics, Vigo University, Spain): efficient algorithms and simulation techniques
- I. Goldhirsch (Technical Faculty, Tel Aviv University, Israel): continuum mechanical description of nanoparticulate systems

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