Karlsruhe Institute of Technology

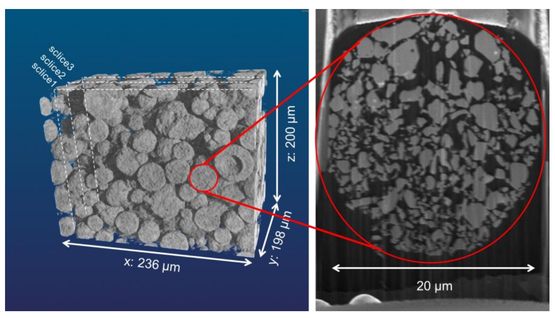
Institute for Applied Materials

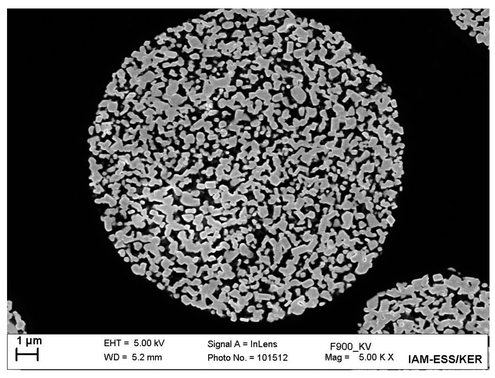
The resistor network method for computing effective transport properties of porous electrodes

Alexandra Pamperin

Motivation

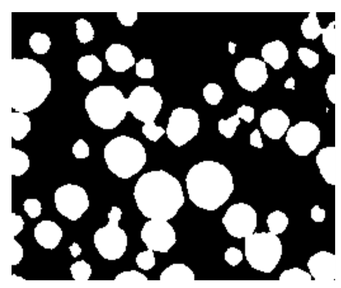
- The granular structure of porouse electrodes has a significant impact on the effective transport properties of the battery cell
- The goal is to optimize the geometry for better transport
- Generating properties necessary for other simulations and models

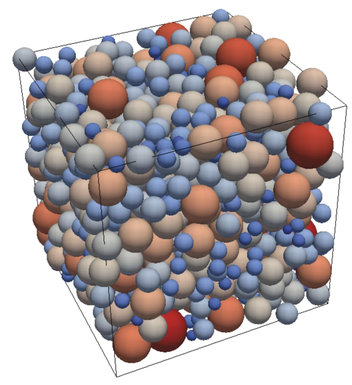


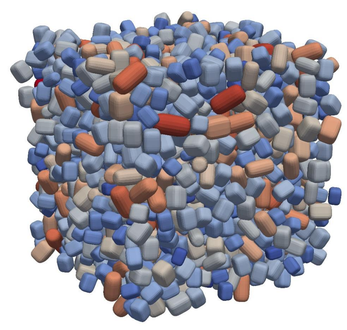


Structure Generation

- Image segmentation and structure reconstruction
- Virtual but realistic structures
- Random close packing algorithm
- Densification through numerical sintering or compression simulation[1,2]
- As of yet particles are only represented by spheres or convex super-ellipsoids



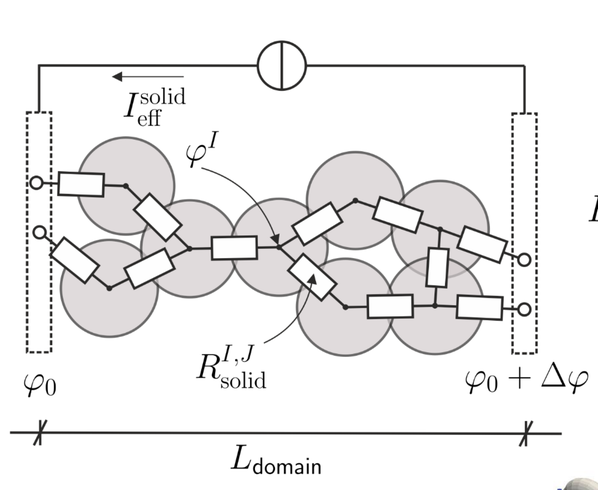


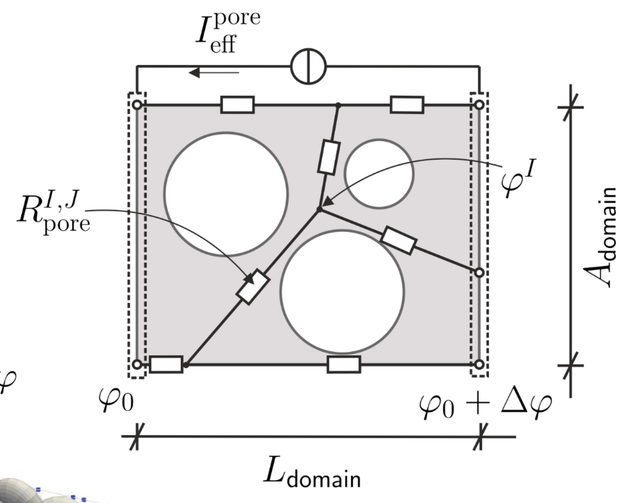


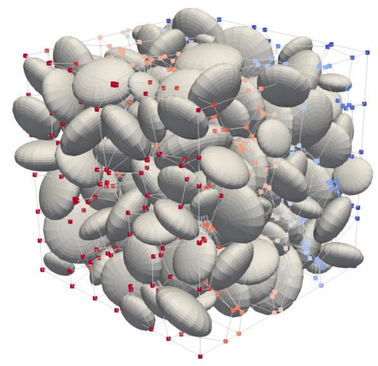
Methodology

- The **Resistor-Network-Method[1]** is used to compute the transport properties of the solid and the porous phase of a particle assembly
- Every particle or pore is associated with a potential
- Every particle contact or pore throat is assigned a resistance
- The potentials can be computed by solving a system of linear equations
- Given the node potentials the effective conductivity is then computed
- The effective transport properties are then given by

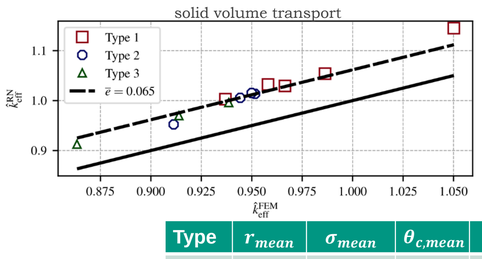
$$\kappa_{eff} = \frac{I_{eff}}{\Delta\varphi} * \frac{L_{domain}}{A_{domain}}$$

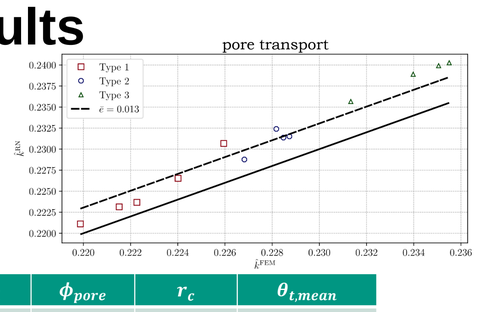






Validation of some results





Type	r_{mean}	σ_{mean}	$\theta_{c,mean}$	ϕ_{solid}	ϕ_{pore}	r_c	$\theta_{t,mean}$
1	1	0	15°	0.655	0.344	0.257	83.35°
2	1	0.1	15°	0.647	0.353	0.242	84.1°
3	1	0.2	15°	0.647	0.353	0.233	84.74°

Outlook

- Numerical sintering of superellipsoids
- FEM validation of effective transport properties for “sintered” superellipsoids
- More detailed contact resistance (particle)
- Impact of local binder distribution
- Mixed conduction paths

Alexandra Pamperin, alexandra.pamperin@kit.edu

1 Birkholz, Oleg (2021): Modeling transport properties and electrochemical performance of hierarchically structured lithium-ion battery cathodes using resistor networks and mathematical half-cell models.
2 Becker, Verena Irene (2022): Modellierung der Mechanik und der effektiven Transporteigenschaften von partikulären Kathoden sowie deren Einfluss auf die elektrochemische Performance von Lithium-Ionen-Batterien. Unter Mitarbeit von Marc Kamlah.

SiMET
POLiS Post Lithium Storage Cluster of Excellence
Bundesministerium für Wirtschaft und Energie → Bundesministerium für Wirtschaft und Klimaschutz