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HiKoMat - Material design of hierarchically structured composite materials for electrochemical storage

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Background

On the occasion of energy transition, new electrochemical storage systems based on **new cell concepts** will be needed to meet today's energy challenges like vehicle **electrification** or **energy storage** from renewable sources. Seen on long terms, battery cells have to be **adjusted to their applications**. Proven concepts are known to be **nano structuring** of active materials and **hierarchical structuring** of electrodes. Furthermore, new **promising material classes** with prospect on enhanced energy and power densities should be investigated concerning these aspects for their application in future.

Abstract

HiKoMat is an interdisciplinary joint project with four key aspects, namely synthesis (**WP1**), imaging (**WP2**), measurement of electronic and ionic parameters (**WP3**) and modelling of cell performance (**WP4**).

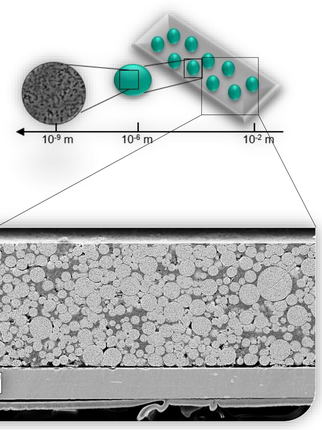
HiKoMat tries first to generate a detailed understanding of the **process-structure-property relationships** in hierarchically structured composite materials and based on this, the **optimization of electrochemical performance** for application is followed.

1 Synthesis and characterization of hierarchically structured composites

[1]Karlsruhe Institute of Technology, Institute for Applied Materials (KWT)
[2]Heidelberg University, Kirchhoff-Institute for Physics

Key aspects

- preparation of hierarchically structured composites by scalable, industry-relevant processes
- establishment of HiKoMat-approach for model system NCM111
- examination of process parameters and process-structure-performance relationships for LIBs



Hierarchically structured electrode

Prospects

- transfer to promising material classes like phosphates, silicates, fluorides
- challenge: low intrinsic conductivities
- approach: carbon coating and polyvalent doping

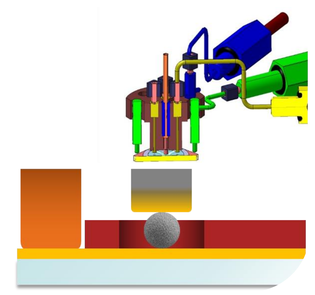
➢ active materials and electrodes are passed to **WP2** and **WP3**

3 Conductivity measurements and electrochemistry on particle and electrode scale

[5]Justus-Liebig-University Giessen, Institute of Physical Chemistry
[6]Justus-Liebig-University Giessen, Institute of Experimental Physics I

Challenges

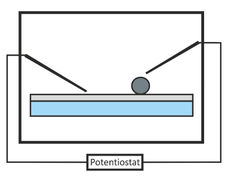
- electronic properties of primary and secondary particles unknown and essential for optimization
- properties vary with shape and surface nature
- no state-of-the-art technique



Lithographic setup

Key aspects

- specification of electronic and ionic conductivities, conductivity paths and contact resistances for nanostructured particles and granule arrangements
- design of meaurement setups for electrochemical investigation



Nanomanipulator setup in SEM

➢ electronic parameters are needed in **WP4** for FEM, DEM and RN calculations

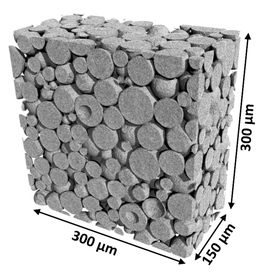
Verification and suggestions for micro- & macro-design

2 3D-imaging and modelling of 3D-structures

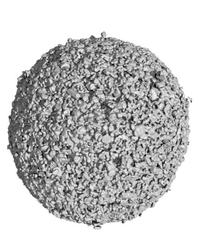
[3]Technical University of Berlin, Institute of Applied Materials
[4]Ulm University, Institute of Stochastics

Key aspects - image analysis of LIBs

- 3D-illustration of the electrode by synchrotron tomography
- microstructure investigation by FIB/SEM
- segmentation of data by algorithms and priming for modelling



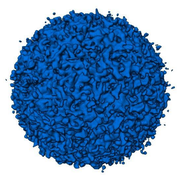
Tomography data



FIB/SEM data

Key aspects - modelling

- quantitative analysis of real structures by stochastic methods
- modelling with parametric approaches and derivation of functional relationship between process and structure
- generation of virtual modified structures



Simulated microstructure

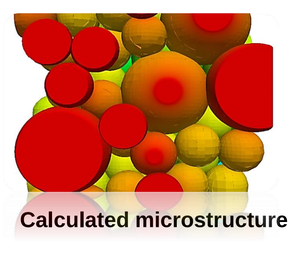
➢ simulated and virtual structures integrated in **WP4**

4 Spatially resolved finite element (FEM)- and discrete element modelling (DEM)

[7]Karlsruhe Institute of Technology, Institute for Applied Materials (WBM)
[8]Heidelberg University, Institute for Applied Mathematics (IWR)

Key aspects - FE simulations of LIB electrodes

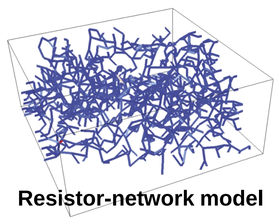
- space-resolved calculation of mass and charge transport (homogenized P2D model and 3D model)
- computation of effective transport properties of macroscopic particles (adaptive cut-cells)



Calculated microstructure

Key aspects - RN and DEM

- compution of effective conductivities of electrodes with resistor-networks (RN) from structure information and effective transport properties
- DEM of calendering process and particle breakdown
- methodology applicable to secondary particle



Resistor-network model

➢ verification of electrochemical performance in **WP1**

➢ virtual electrode design in collaboration with **WP1**

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Gefördert durch:
Bundesministerium für Wirtschaft und Energie
Projektträger Jülich Forschungszentrum Jülich