GeoDict
The Digital Material Laboratory

DELFIN

Delfin – Development of a validated software tool for All-Solid State Battery materials
Understanding the material-property relationships for electrode design through digital material research & development.

In the public research project **DELFIN** we strive to develop a validated software tool for digital R&D of All-Solid-State Batteries (ASSBs). Our project partners comprise of both academic and commercial partners: Experimental design of ASSB cathodes and electrochemical experiments are conducted at **Justus-Liebig University in Giessen**, digitalization of cathode structures using new approaches in µ-CT 3D scans are provided by **RJL Micro&Analytics**. Our partner group at **University Ulm** develop stochastical structure generators to model ASSB cathodes. At Math2Market, we combine the developments into the BatteryDict and Import tools, validate the results with experiments and provide a product ready for the digital design of ASSBs.

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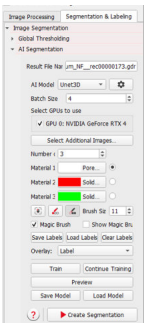
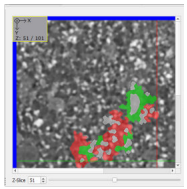
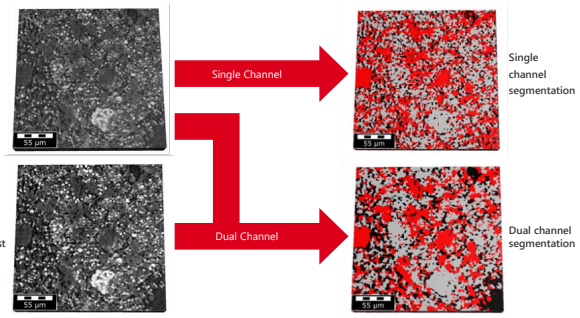
RJL Micro & Analytic





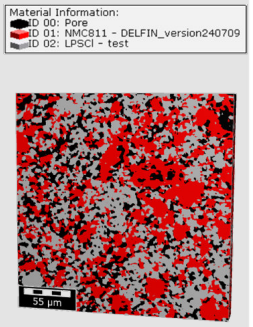


Digitalize Cathode Structures

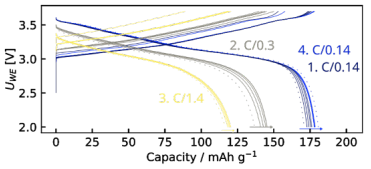
µCT data is commercially available, but resolution is at the limit of usability for ASSB applications

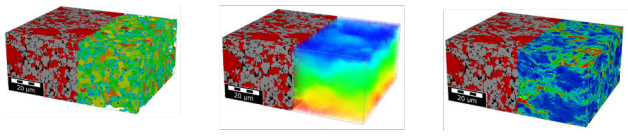
- **Standard:**
  - Good topographical resolution
  - Resolution up to 0.1 µm possible
- **Free Field Phase Contrast:**
  - Material contrast / chemical composition
  - High contrast for materials and background

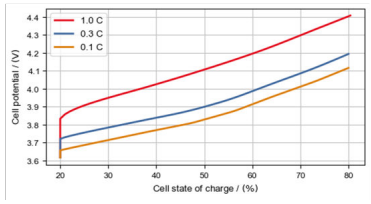
Observation
- Detailed texture in Standard reconstructed image
- High contrast between foreground and background and materials in Free Field Phase Contrast image



Justus-Liebeig-University Giessen





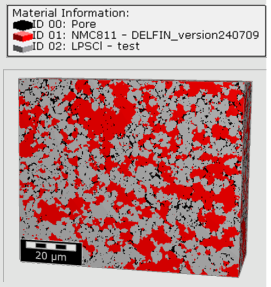


Geometric parameters	Transport parameters	Operation of batteries
■ Porosity ■ Pore size distribution ■ Grain size distribution ■ Surface area ■ Length of contact lines ■ Tortuosity	■ Conductivity ■ Diffusivity ■ Lithium concentration ■ Path of single particle	■ Charge curve for variable charge rates ■ 3D Li-concentration during operation with fully resolved simulation ■ Fast simulation using a homogenized model (pseudo-2D Newman model) ■ Instant estimation of charge curve

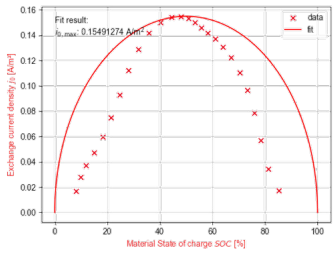
Analyze cathode structures and validate simulation results

BatteryDict slows for solid electrolytes and configures the solver equations accordingly:

- Diffusion and migration terms are not required regarding ASSBs.
- Since the transfer number is always t+=1, charge conservation and electroneutrality term are simplified.
- Accounting for the exchange current between active materials and solid electrolytes is now implemented in the material database
- New materials such as LPSCl are shipped with GeoDict 2025 to allow ASSB simulations in BatteryDict.

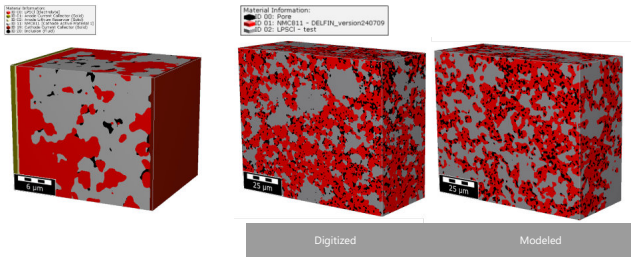


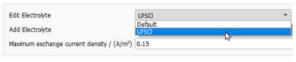
University Ulm



Exchange Current Density plotted against the State of Charge (SOC) NMC811-LPSCl

Source: Anja Bielefeld et al 2022 J. Electrochem. Soc. 169 020539





Interface between electrolyte and active material

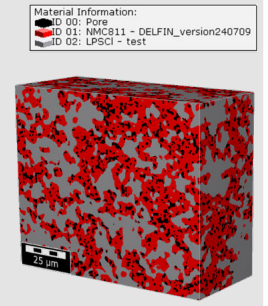
$$i_{se} = 2\, i_{0,max} \sqrt{\left(1 - \frac{c_s}{c_{max}}\right) \frac{c_s}{c_{max}} \sqrt{\frac{c_e}{c_{e,equ}}}} \cdot 2 \sinh\left(\left(\varphi_s - \varphi_e - U_0\right) \frac{F}{2RT}\right)$$

Interface between electrolyte and lithium reservoir

$$i_{se} = i_{0,max} \sqrt{\frac{c_e}{c_{e,equ}}} \cdot 2 \sinh\left(\left(\varphi_s - \varphi_e - U_0\right) \frac{F}{2RT}\right)$$

Modelling ASSB cathode structures

- ASSB cathode generator GeoApp will be available in GeoDict
- GeoApp to carry out the virtual design of ASSB cathodes using a parametric model
- New materials (like LPSCl) available in the GeoDict material database
- Publication with University Ulm has been submitted!



DELFIN enhances the design of ASSB materials
- from segmentation over structure analysis to new structure generators -

Our project partners:

Justus-Liebeig-Universität Giessen
- Dr. Anja Bielefeld
- René Rekers

RJL Micro & Analytic
- Dr. Markus J. Heneka
- Dr. Jochen Joos

Universität Ulm
- Prof. Volker Schmidt
- Dr. Orkun Furat
- Sabrina Weber
- Anina Dufter

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