Machine learning for structure reconstruction and particle sizing of battery electrodes

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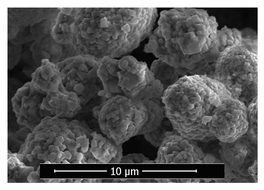
Introduction

- DigiBatMat project enables the digital description of lab- and pilot-scale battery production and characterization data and links battery material, process, and analysis to generate additional knowledge
- Focused ion beam (FIB) and scanning electron microscope (SEM) are used to reconstruct the 3D structure of lithium-ion battery cathodes
- Varying acceleration voltages alters the information depth of the segmentation
- Multi-kV tomography data is used to train the machine learning algorithm for this material combination
- Consistent output of quantified data and linkage with the structured process parameters in the digital platform enables fine-tuning of production processes and comparison analysis
- Electrode processing parameters, electrode properties, and the microstructure analysis are linked via the DigiBatMat platform “DataCharge.io”

Materials

Cathode active material:

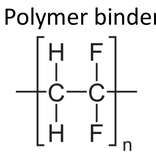


Lithium-Nickel-Cobalt-Aluminium-Oxide (NCA)

Conductive additive:

C65-Carbon black (CB)

Polymer binder:



Polyvinylidene fluoride (PVDF)

Slurry

Calendered cathode

Process variation

Processes:

1. Calendering

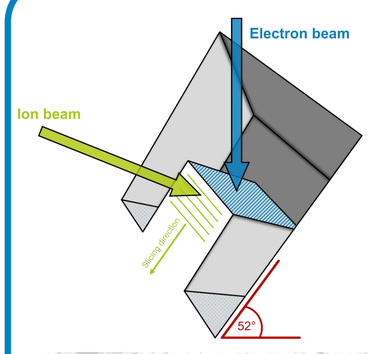
- Particle compaction
- Pore space distribution

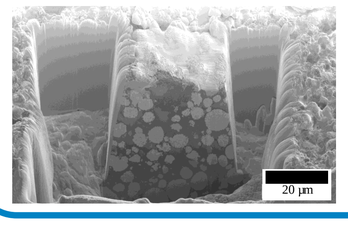
2. Wet mixing

- Dispersion state
- Agglomeration
- Aggregate size distribution

Microstructure:

Method

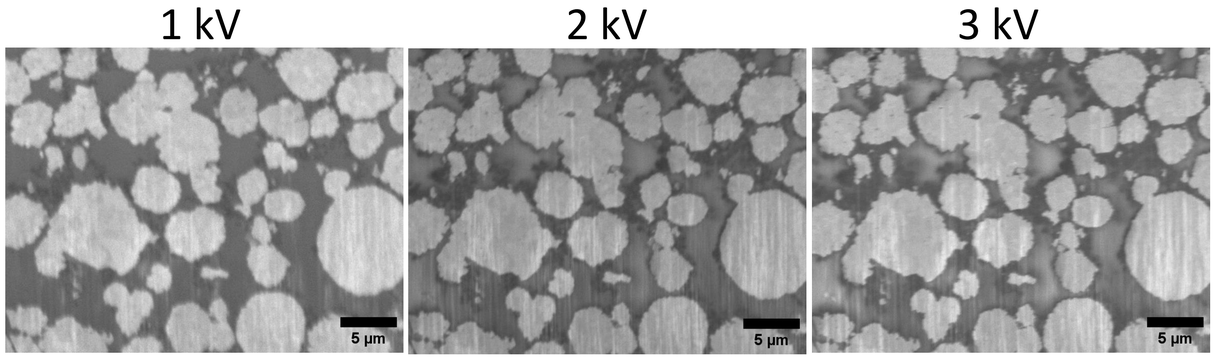




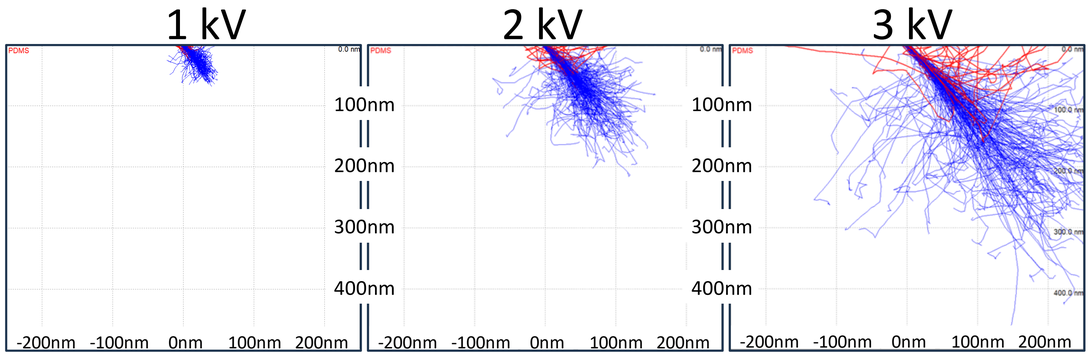
- Cathodes are pore-space backfilled with silicone
- Secondary electron images for highest resolution
- x/y/z resolution set by electron + ion beam parameters
- Resolutions down to 10 nm possible

Left: Cross section of li-ion cathode

Contrast and resolution in SEM

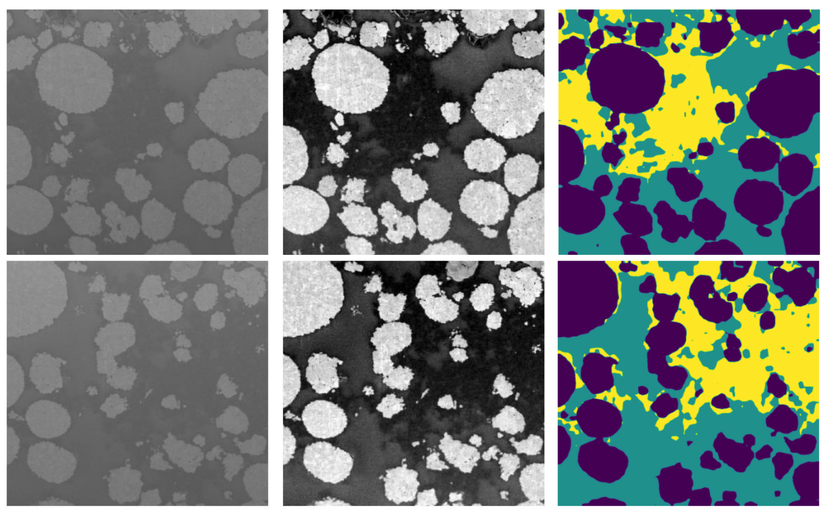


Effect of acceleration voltage in low-kV SEM:
Decreasing the acceleration voltage increases the resolution but introduces artifacts (charging, grey scale fluctuations, more pronounced curtaining)



Effect of acceleration voltage on information depth:
For single slice information depth in pore-space backfilled with polymers, the electron acceleration voltage should be at lowest possible kV

Machine learning approach

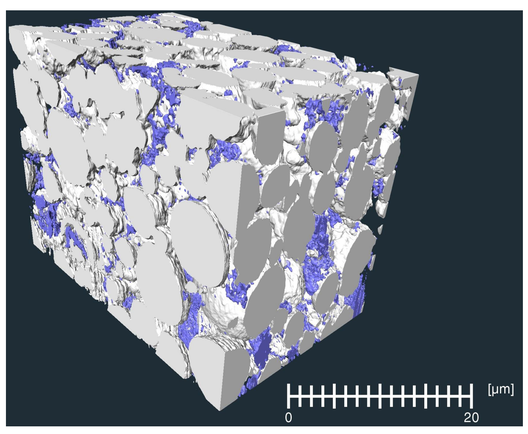


- Image preprocessing pipeline mitigates illumination changes and other imaging artifacts
- Combine classical methods for denoising and contrast correction with a novel surface fitting approach to remove macroscopic brightness changes
- Segmentation of the pre-processed images is performed using a neural network, that is trained specifically for these images
- Multi-kV data of same images increases the quality of the ML model

Left Original; **Middle** Preprocessed; **Right** Phase-Segmentation

Reconstruction

The labeled data is used to quantify phase properties of the electrode and is linked in the platform to processing parameters and electrode properties



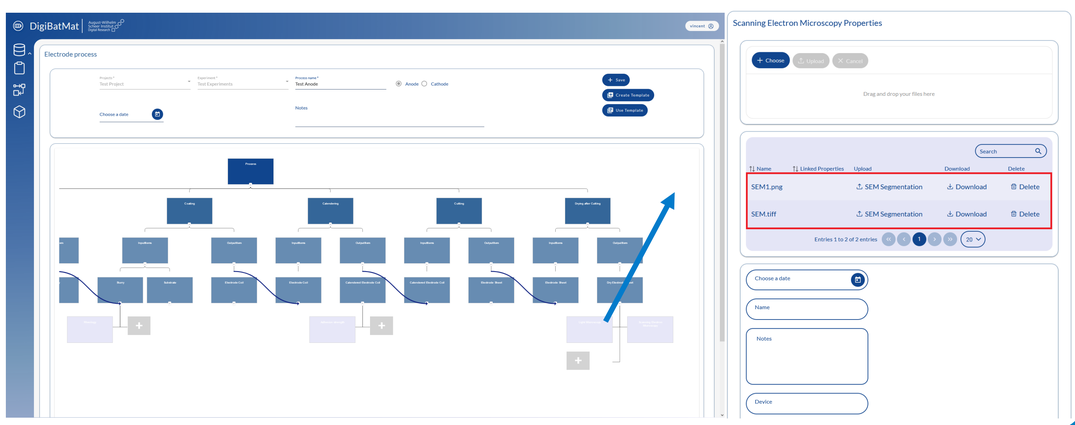
Phase properties:

- Volume fractions of materials
- Active material dispersion
- Tortuosities of the electronic (CB) and ionic (pore space) conductive network
- CB Microstructure

Above: Example reconstruction electrode tomography

Implementation into DataCharge.io

- The segmentation pipeline is a feature in the DataCharge.io platform
- Machine settings and preprocessing parameters will be set directly via the characterization method properties
- After uploading the SEM images to the platform, the user can start the pipeline with a single click and the results are automatically stored within the created characterization method



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