Reconstruction of the active material, binder and pore space of a $LiCoO_2$ Li-ion battery cathode

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In the reported work, we reconstruct a $LiCoO_2$ cathode, for the first time differentiating between all three constituents: (i) active material, (ii) binder and (iii) pore space for this specific material. We apply a hybrid method of manual and grey-scale threshold segmentation for reconstruction. The reconstructed images are assembled to a three-dimensional geometry.

INTRODUCTION

Till now most models predicting lithium-ion battery behaviour are based on the porous-electrode theory [1]. Focused ion-beam scanning / electron microscopy (FIB/SEM) [2] can be employed to study a given microstructure by removing thin layers of electrode material and combining images of each layer to produce a three-dimensional reconstruction of the respective electrodes thus replacing the porous-electrode theory with a more realistic description of microstructure. This technique was utilized to study the $LiCoO_2$ cathode of a lithium-ion battery, differentiating between the active material and a combined binder and pore phase [3]. Like Wilson et al. [3], we focus on a $LiCoO_2$ cathode. Unlike them, we differentiate between all three constituent parts - (i) the active material, $LiCoO_2$, (ii) the binder and (iii) the pore space - by applying a hybrid method of manual and grey-scale threshold segmentation.

EXPERIMENTAL

To obtain the electrode material used in this work, a new VARTA LIC 18650 WC lithium-ion battery was unsealed and dismantled. After evaporation of the electrolyte, a piece was extracted from the cathode and prepared for FIB/SEM. With the help of an FEI Quanta three-dimensional dual-beam FIB-SEM at Fraunhofer IZM, Berlin, a cavity was cut into the sample as a starting point and subsequently one side of the cuboid was ablated slice by slice, while the SEM, with an angle of 38° relative to the sample surface, generated one image per slice.

IMAGE PROCESSING

In a first step, the images were aligned to compensate for both global sample movement due to vibrations and temperature-induced contraction and expansion and the angled REM. The images were cropped to remove unwanted fringe areas, generating a stack of 200 images describing a cuboid which measures 20.02 μm x 18.13 μm x 12.4 μm.

The segmentation was performed on an image-by-image basis by generating a specific histogram of each image and pre-segmenting the three phases by threshold values given by minima between the overlapping intensity peaks of $LiCoO_2$ and binder phases and left of the binder phase peak. Where required, this segmentation was corrected manually by comparing the pre-segmented images with the original image and its respective neighbouring images (Fig. 1).

Finally the segmented images were assembled to create a 3D reconstruction of the sample (Fig. 2).

CONCLUSION AND OUTLOOK

In the reported work, the three-dimensional reconstruction method was utilized for the first time to identify and differentiate between all three phases of the $LiCoO_2$-based cathode of a Li-ion battery. In future work we will use this reconstruction to generate parameters to support the data basis of homogenized cathode models.

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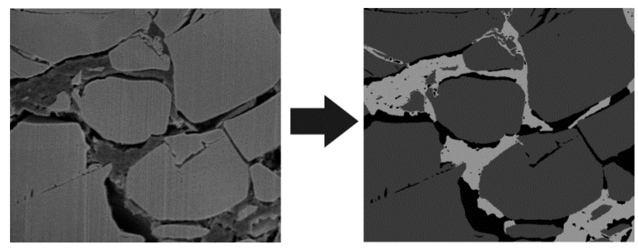

Figure 1: Segmentation of an SEM image. Active material (dark grey), binder (light grey) and pore space (black) are specified by their respective color.

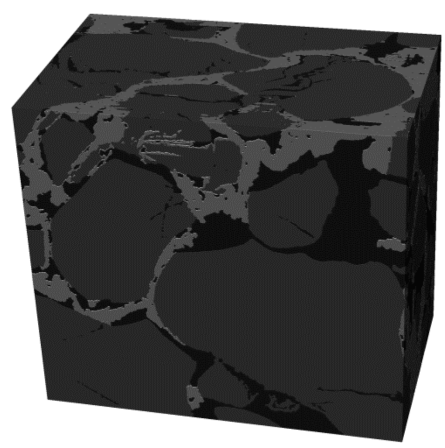

Figure 2: 3D reconstruction of the sample. Active material (dark grey), binder (light grey) and pore space (black) are specified by their respective color.

REFERENCES

[1] J. Newman and W. Tiedemann, *AIChE Journal*, 21, 25-41 (1975).
[2] L. Holzer, F. Indutnyi, P.H. Gasser, B. Munch and M. Wegmann, *Journal of Microscopy*, 216, 84-95 (2004).
[3] J.R. Wilson, J.S. Cronin, S.A. Barnett and S.J. Harris, *Journal of Power Sources*, 196, 3443-3447 (2011).