Calculation of tortuosity in a Li-ion battery cathode based on FIB/SEM tomography

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Tortuosity is regarded as one of the most important parameters to characterize a porous medium [1]. In the past, the tortuosity of Li-ion battery cathodes was usually calculated by expressing it as a function of the porosity via the Bruggeman equation. However, there is considerable doubt concerning the accuracy of this relation. We present a new method to calculate tortuosity. The starting point is the 3D reconstruction of a $LiCoO_2$ cathode created from FIB/SEM images with three phases, the active material domain, carbon-binder domain and pore space [2]. Pore size distributions, as determined by this work, suggest that a significant number of pores in the carbon-binder domain cannot be resolved by FIB/SEM. This conclusion is additionally supported by experimental data generated by Stephenson et al. [3]. To account for this, we propose a nanoporous carbon-binder domain with the following experimentally derived parameters [3]: i) 65% porosity. ii) Li-ion diffusivity or conductivity of 5% compared to the pore space filled with electrolyte. We compute joint effective diffusivities for pore space and carbon-binder domain for all three spatial directions. From this we calculate tortuosity values of 4.2 (x direction), 6.1 (y direction, the through-plane direction) and 5.7 (z direction). These values are consistent with experimental values for Li-ion cathodes reported previously [3].

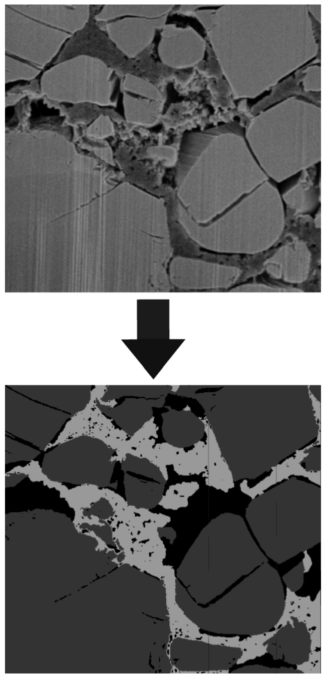

Figure 1: *3D reconstruction by FIB/SEM tomography with a subsequent segmentation step enables the calculation of tortuosity. Pore space (black), active material domain (dark grey) and carbon-binder domain (light grey) are specified by their respective color.*

[1] M. Doyle, J. Newman, A.S. Gozdz, C.N. Schmutz, J.M. Tarascon, *Journal of The Electrochemical Society* 143 (1996) 1890.

[2] T. Hutzenlaub, S. Thiele, R. Zengerle, C. Ziegler, *Electrochemical and Solid-State Letters* 15 (2012) A33.

[3] D. E. Stephenson, B.C. Walker, C.B. Skelton, E.P. Gorzkowski, D.J. Rowenhorst, D.R. Wheeler, *Journal of The Electrochemical Society* 158 (2011) A781.