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MULTI-SCALE MODELLING OF A LI-ION BATTERY ELECTRODE WITH ALIGNED PORES

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There is a growing interest in increasing the accessible capacity of Li-ion battery electrodes without compromising the power. This is a challenging task since as the electrode thickness increases, the ionic transport in the electrolyte becomes limiting. In order to facilitate ionic transport, we investigate the effect of the introduction of micro-channels aligned along the electrode thickness by using a multi-scale modelling approach.

A volume-averaged electrochemical model is developed to take into account charge transport in concentrated solution, charge transfer at the solid/electrolyte interface, and electron migration and lithium diffusion in the electrode material [1]. Carbon nanoparticles are embedded within the electrode material to increase the effective electronic conductivity, which is evaluated through TauFactor [2] by simulating random dispersions of nanoparticles.

A multi-scale optimisation strategy is adopted: at the micro-scale, the volume fraction of carbon nanoparticles is optimised in order to enhance the effective electronic conductivity without compromising the electrode capacity; at the electrode level, the diameter, pitch and length of micro-channels are varied to maximise the power density. Results show that the electronic conductivity is significantly increased as soon as percolation of the carbon nanoparticles is achieved. At the electrode level, as long as the volume fraction of micro-channels is constant, smaller pores lead to higher current densities.

Finally, a positive electrode fabricated via freeze-casting according to optimised geometric parameters identified by the model is produced, tested and reconstructed with 3D X-ray tomography. The difference between model predictions and real electrochemical performance may in part be attributed to the pore morphology of the actual sample, which is more complex than the prismatic forms captured in this model.

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