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Finite difference heterogeneous modelling of Li-ion composite electrodes based on nano-scale X-ray computed tomography

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Lithium ion intercalation leads to volume changes of ~10% in graphite electrodes, and ~400% in Si based electrodes. SEM, TEM and NMR have all been used extensively in electrode analysis, however they only allow 2D samples to be analysed, meaning 3D volumetric properties are missed. X-ray tomography techniques are favoured by the author as they are a non-destructive imaging platform whilst also being able to provide the multiple length scales required. Diffusion has traditionally been measured experimentally through the use of a diffusion cell, however with advances in CFD and FEA, and imaging techniques, more detailed investigations can be carried out [1].

The Bruggeman equations correlate tortuosity factors of porous media with their porosity and are commonly used in modelling li-ion transport through a flooded porous electrode. Newman-type models (e.g. Newman pseudo 2D (P2D)) often use this correlation. The Bruggeman relation is found to only be valid in situations where the insulating phase is present in a low volume fraction and represented by random, isotropic spheres. It cannot account for directional differences which arise from non-spherical particle packing. Applying this correlation to heterogeneous structures (e.g. battery electrodes) is invalid and more complex approaches are required to sufficiently characterise the transport properties of the material and its resulting tortuosity factor [2].

This work develops a parallel (MPI) code that calculates tortuosity factor, driven by real electrode microstructure through x-ray tomography obtained voxel sets. These voxel sets are overlaid with finite-difference grids which are used as numerical domains to solve the relevant partial differential equations. This code performs a similar function to the open-source software package TauFactor [3]. However, this is just the first step on the path to develop an open-source software package to solve fully 3D multi-physics models for electrodes (electrochemical, thermal and electrical). The methodology is to ultimately develop a software package that requires minimal human input in order to automate the workflow from electrode microstructure to battery performance.

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