Batteries for Electric Vehicles - Cathode Microstructure Design

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Abstract

Due to the rapid growth of the electromobility market much effort currently is being put into investigating electric vehicle batteries. Optimizing the microstructure of the cell components is playing an important role in extending range, enhancing fast charging capabilities and reducing aging of batteries, making the microstructure the focus of current research.

When it comes to modeling the microstructure, Newman's P2D model enjoys widespread use. However, it is severely limited in that it only resolves the microstructure in one Cartesian dimension and in the radial coordinate of the secondary particles. Therefore, three dimensional models have been developed to investigate the microstructure in further detail, i.e. composition, size and spatial distributions of the secondary particles. However, such simulations typically treat secondary particles as consisting of a homogeneous material with isotropic properties. Actually secondary particles exhibit a sub-microstructure since they consist of primary particles having various sizes, shapes and orientations.

We modeled secondary particles with various sub-microstructures and then investigated their behavior using the 'Batteries and Fuel Cells' module in COMSOL Multiphysics®. We applied so called 'Lithium-Ion Battery' and 'Transport of Diluted Species' physics to obtain insights into the electrochemical processes taking place in a single battery cell. Our COMSOL model is three dimensional and makes use of a half-cell configuration, in which a single secondary particle, representing the active material of the cathode, and a lithium counter electrode are electrically charged. The electrodes are separated by an electrolyte which is attributed the effective properties of a separator filled with electrolyte.

Applying this model in COMSOL Multiphysics® we obtain insights into lithium distribution and flux during charging and discharging a battery cell.

Figures used in the abstract

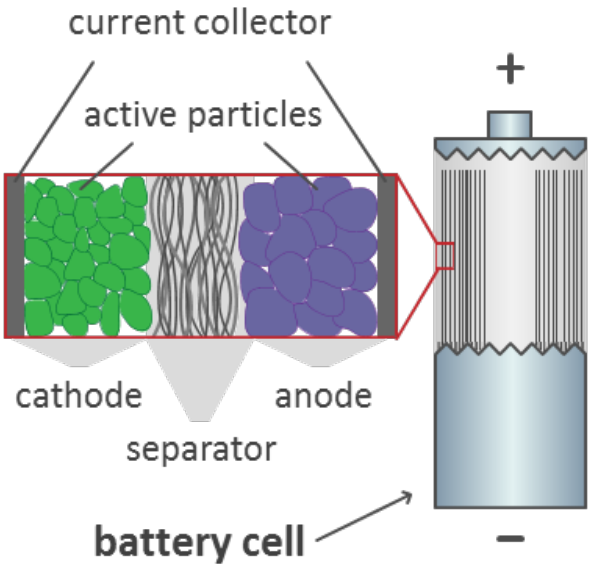

Figure 1: Sketch of a battery cell and its microstructure.