Batteries for Electric Vehicles – Cathode Microstructure Design

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INTRODUCTION: When it comes to modeling battery cells, Newman's P2D model enjoys widespread use. However, it is limited in that it treats secondary particles as spheres of homogeneous, isotropic material. Actually, secondary particles exhibit anisotropic material properties which result from their layered atomic structure. Therefore we investigate the impact of planar lithium diffusion in secondary particles on their capacity.

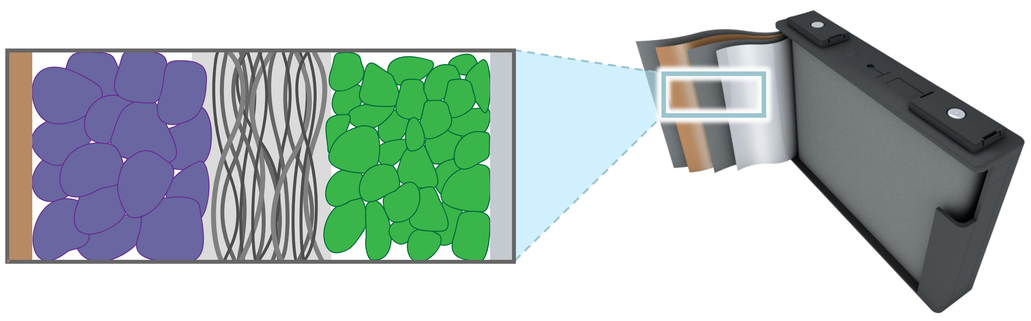

Figure 1. Microstructure of an electric vehicle battery cell

COMPUTATIONAL METHODS: We model single secondary particles and then investigate their behavior using the 'Battery and Fuel Cells' module in COMSOL®. We apply so called 'Lithium-Ion Battery' and 'Transport of Diluted Species' physics to obtain insights into the electrochemical processes taking place inside a single particle. The geometry of our COMSOL® model is shown in figure 2. It 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 model is three dimensional and takes anisotropic diffusion of the active material into account and further allows to rotate the local coordinate system of the single particle.

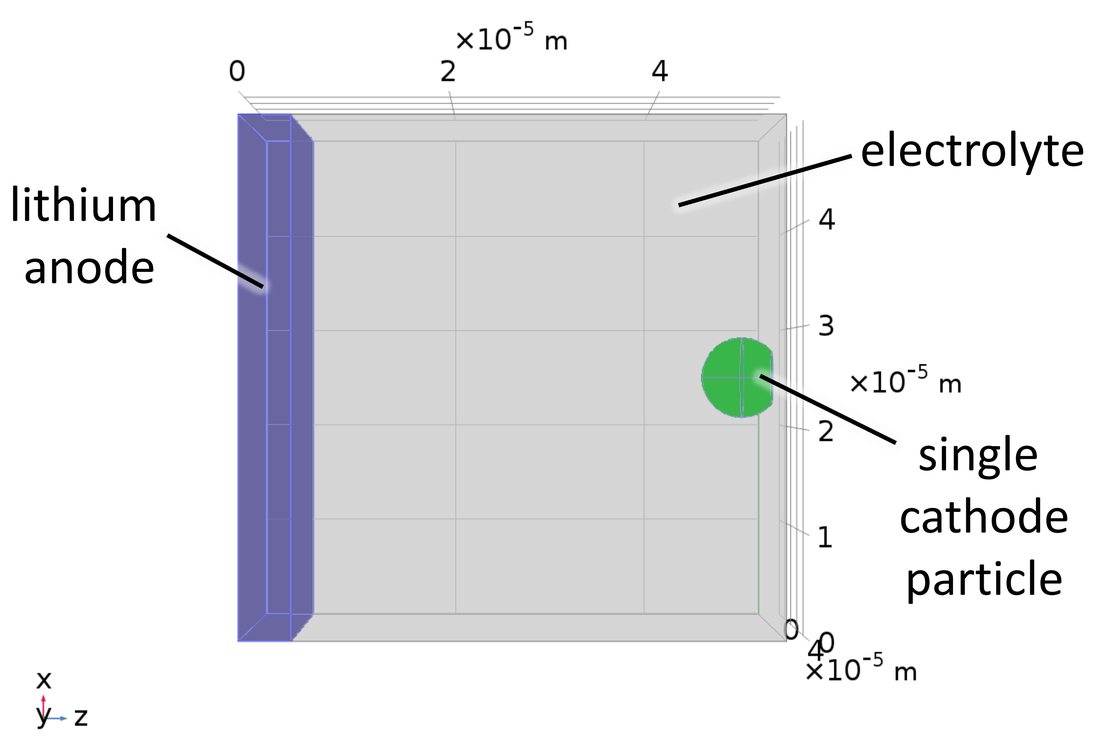

Figure 2. Geometry of the COMSOL model

RESULTS: Compared to the isotropic case planar lithium diffusion results in a significant capacity loss. Lithium accumulates faster in the regions where the circular diffusion planes become smaller (figure 3). Further, the orientation of these planes affects the capacity by roughly ten percent (figure 4).

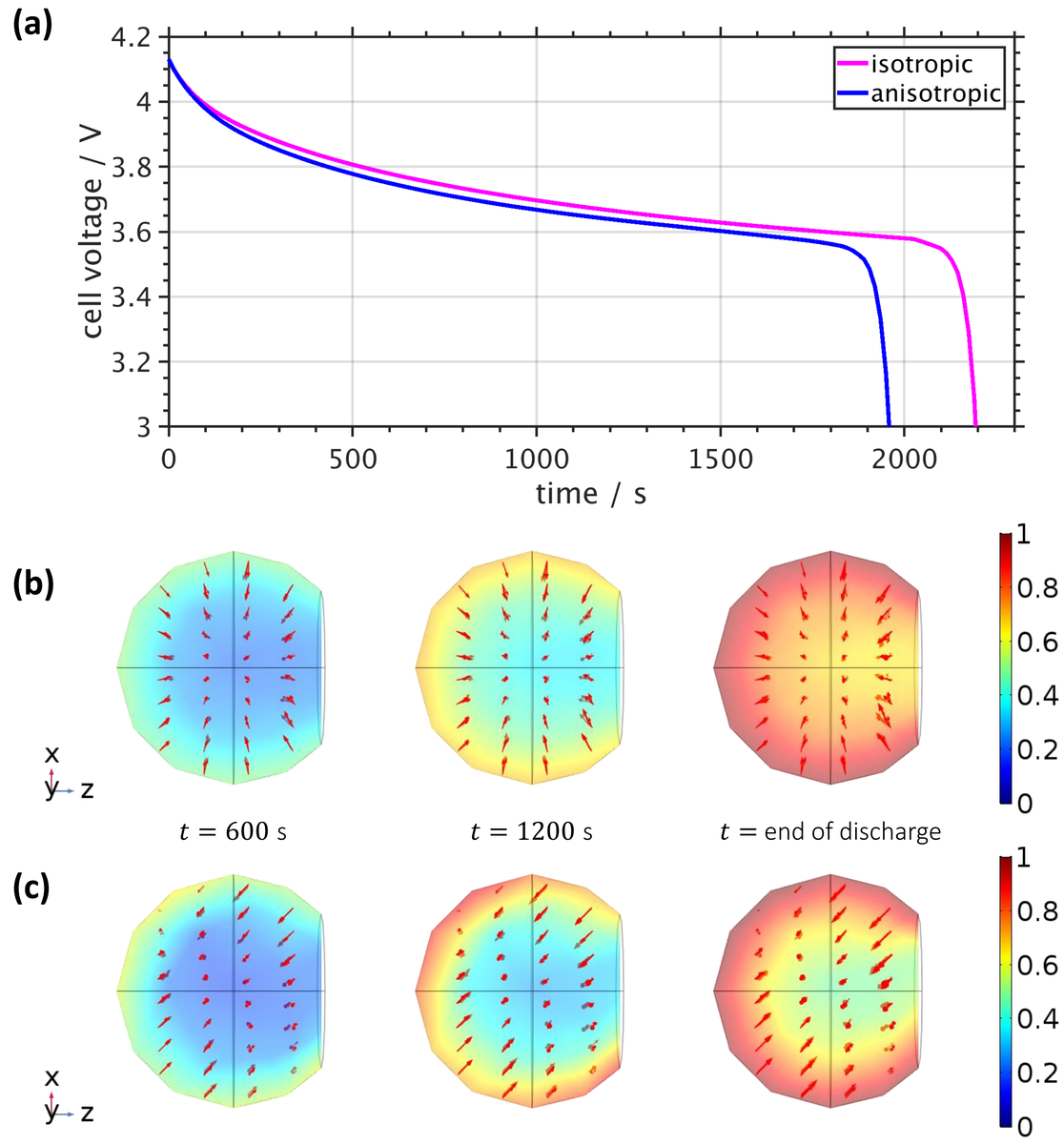

Figure 3. Discharge curves **(a)** of a secondary particle with isotropic and anisotropic (planar) diffusion. Time series of the state of charge and the lithium flux of the isotropic **(b)** and the anisotropic **(c)** case

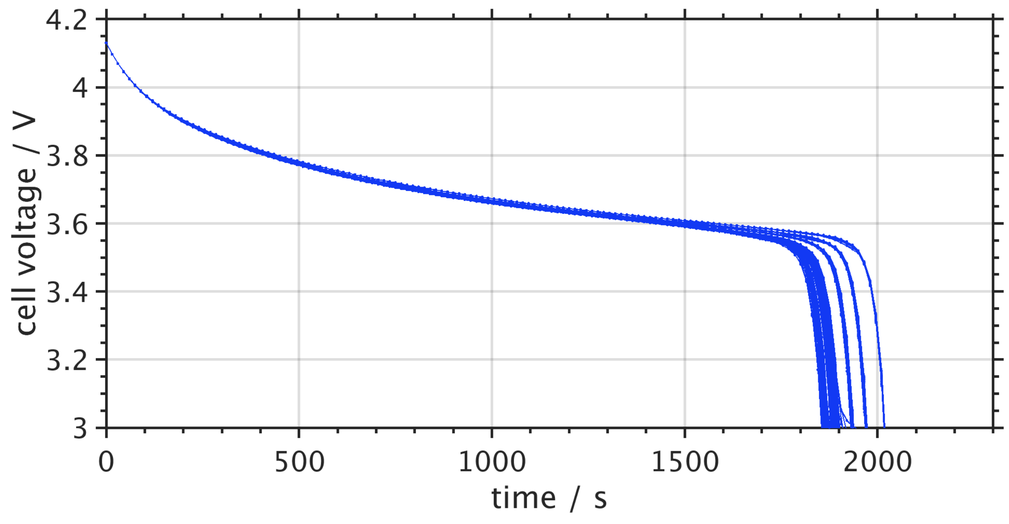

Figure 4. Discharge curves for varying orientations of the diffusion planes

CONCLUSIONS: At a C-rate of 1 C planar lithium diffusion affects the capacity of secondary particles severely. Thus, three dimensional models are supposed to incorporate anisotropic diffusion, which is not possible in Newman's P2D model.