Modelling of Lithium Ion Batteries with Silicon Anode and Ionic Liquid Electrolyte

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Modelling and simulation play an important role in the development of safer, higher performing lithium-ion batteries. Our continuum model combines mechanical effects on the electrode side with our novel transport theory for strongly correlated electrolytes[1]. This thermodynamically consistent transport theory couples chemical, electrical and mechanical contributions. It was validated in the bulk phase and at interfaces where it captures effects such as crowding and overscreening[2]. For certain electrode active materials lithium intercalation causes large deformations. The resulting coupled mechanical and chemical stresses are incorporated on the electrode side. Lithium-ion transport throughout a cell is thus captured in a macro-homogenized 1d+1d model.
We apply our model framework to a lithium-ion battery consisting of a silicon nanowire anode, an ionic liquid electrolyte and a standard lithium cobalt oxide cathode. We model the nanowire structure of the silicon anode in a cylindrical geometry. Full cell simulations are carried out with MATLAB.
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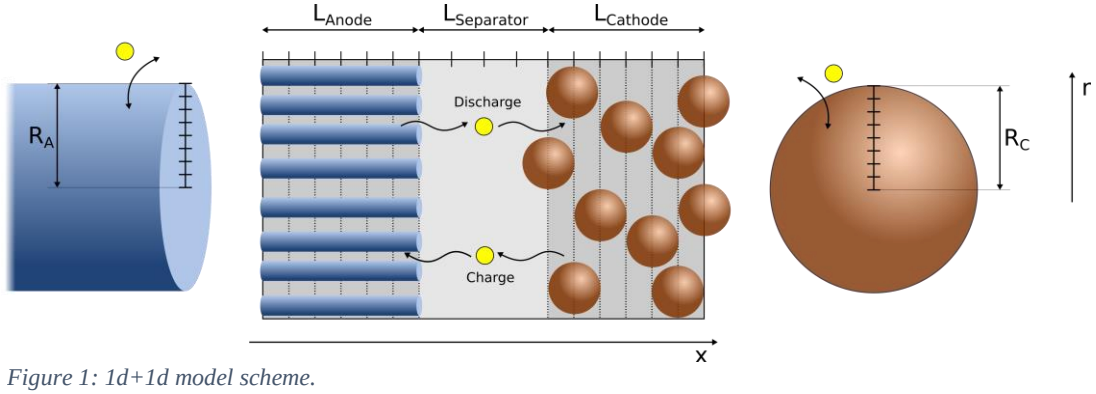

Figure 1: 1d+1d model scheme.

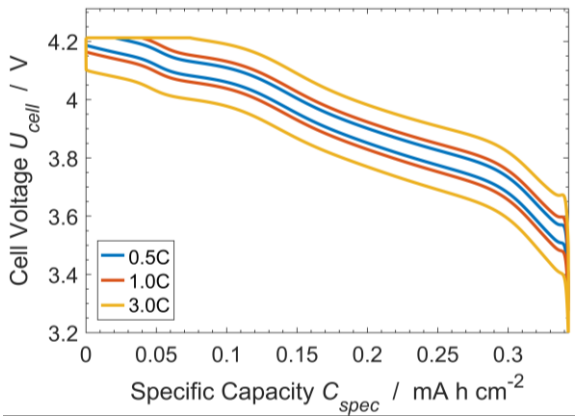

Figure 2: Discharge-charge curves for different C-rates.

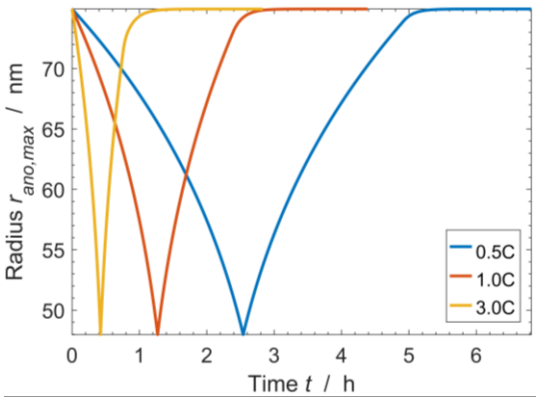

Figure 3: Change in the nanowire radius during one cycle at different C-rates.

References:
[1] M. Schammer et al., *J. Electrochem. Soc.*, **2021**, *168*, 026511.
[2] V. Hoffmann et al., *Phys. Chem. Chem. Phys.*, **2018**, *20*, 4760.