Abstract for oral presentation

Modeling of structured electrodes in lithium-sulfur batteries

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Due to their high theoretical capacity lithium-sulfur batteries (Li/S) are envisioned as next-generation storage technology for electric vehicles [1]. However, several challenges obviate a successful commercialization of the battery. Most of them are related to the high solubility of intermediate polysulfide species and the resulting so-called 'shuttle effect'. The transport of polysulfides between positive and negative electrode causes a decay of capacity and low coulombic efficiency upon cycling. Experimental studies [2] demonstrate that nano-structuring of carbon/sulphur composite electrodes significantly improves the cyclability of the battery. Micro-porous particles [3], hollow carbon spheres (HCS) or carbon nano tubes (CNTs) are used to encapsulate the sulphur and to prevent transport of polysulfides to the anode.
In our contribution we present results of a detailed 1D single particle continuum model describing reaction and transport inside a representative spherical particle [4], [5]. On the surface we assume that only lithium ions are able to enter and leave the particle. This relatively simple model gives some interesting insights on the behavior of the particle during battery operation. Most prominently, we identified an additional overpotential during discharge resulting from the transport of Li ions against a concentration gradient into the particle.
In a following step we couple the single particle model to a macroscopic model of a full battery cell. Results of the 1+1D full cell simulations are parameterized and validated based on experimental data [3]. Systematic parameter studies reveal the influence of novel electrode geometries on battery performance and are able to guide future improvements in electrode design.

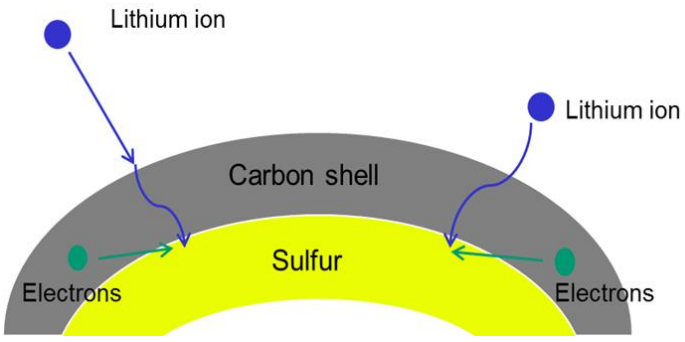

Figure 1: Schematic depiction of a lithium-sulfur particle with carbon shell.

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[2] Ji, X. et al. *Nat. Mater. 244 (*2009), pp. 500–506.
[3] Thieme, S. et al. *J. Mater. Chem. A* 1 (2013), pp. 9225.
[4] Fronczek, D. N. et al. *J. Power Sources 244 (*2013), pp. 183–188.
[5] Hofmann, A. F. et al. *J. Power Sources 259 (*2014), pp. 300–310.