

Modeling of adsorption processes at nanostructured cathodes in lithium-sulfur batteries

Jessica Lück^{1,2,3} and Arnulf Latz^{1,2,3}

*¹German Aerospace Center (DLR), Institute of Engineering Thermodynamics,
Stuttgart , Germany*

²Helmholtz Institute Ulm (HIU), Ulm , Germany

³University of Ulm, Institute of Electrochemistry, Ulm , Germany

Due to its high theoretical energy density lithium-sulfur batteries are one of the most promising candidates for future energy storage. This position is further based on low costs, an intrinsic overload protection, non-toxicity and the natural abundance of its compounds [1]. Nevertheless even after 5 decades of research lithium-sulfur cells are still far away from a commercialization. All occurring challenges in the operation of lithium-sulfur batteries are associated with intermediate species, which are produced when lithium reacts with sulfur [2]. These lithium polysulfides differ in their chain length and their solubility. Soluble polysulfides generate a redox shuttle between cathode and anode, while insoluble polysulfides precipitate on the anode. This leads to a reduction of active sulfur and to a corrosion and polarization of the anode. One strategy to overcome this is a structuring of the cathode to retain soluble lithium polysulfides [3].

We present a thermodynamically consistent continuum model for nanostructured sulfur carbon composite cathodes. All polysulfides are assumed to be contained in carbon particles. Particular emphasis is put to the adsorption of Li ions on the carbon surface and covers the influence of the electrochemical double-layer. The surface effects are modeled from electrostatic considerations only, without assuming structural properties of the double-layer. Therefore, the model allows us insight into the chemical and physical processes at the electrode-electrolyte interface as well as their influence on the operation of a Li-S battery.

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