Experimental and Theoretical Analysis of Products and Reaction Intermediates of Lithium-Sulfur Batteries

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The identification and quantification of species involved in the electrochemical reactions of lithium-sulfur batteries are still unclear and controversial aspects of the investigation of these cells. However, a deeper understanding of the system is crucial to improve the capacity and cycling stability of the cell.
In this work, the reduction process of sulfur in a lithium-sulfur battery was studied using UV-Vis spectroscopy under argon atmosphere [1]. Absorbance maxima of dissolved sulfur and polysulfide species were determined at various concentrations. Reference solutions of polysulfides reduce the λ_{max} in the UV-region with decrease of polysulfide order. This tendency is also observed between 25–75% depth of discharge due to the progressive reduction of polysulfides in the electrolyte. Because the application of UV-Vis spectroscopy alone does not provide a complete overview of the distribution of all species during cycling, we present a comparison between the output of a physicochemical model [4] with experimental data obtained from UV-Vis spectroscopy [1], X-ray diffraction [2] and electrochemical impedance spectroscopy [3]. The model affirms that the highest concentration of polysulfide is observed when all sulfur has been dissolved. In the tested cells, this occurs at around 37% DOD (450 $Ah \cdot kg_S^{-1}$). A significant concentration of polysulfides is confirmed at the end of discharge which is of significant importance for improving the cycling stability of lithium-sulfur cells.

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