Lithium/Sulfur Batteries: An Elementary Modeling Approach

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The lithium/sulfur (Li/S) battery is a promising system for energy storage. Its energy density (up to 2.6 kWh/kg) is the highest of all "closed-system" batteries known [1]. The global reaction of this type of cell is

$$S_8 + 16\,Li \rightleftarrows 8\,Li_2S \ ,$$

yielding 3400 kJ/mol and a open-circuit voltage of ~2.2 V. However, due to the complex redox chemistry of sulfur, numerous soluble intermediate species are formed during discharge, including S_8, S_8^{2-}, S_6^{2-}, S_4^{2-}, S_2^{2-} and S^{2-}. The large number and different properties of those intermediates represent a major challenge in understanding Li/S electrochemistry.

A computational model of the Li/S cell is presented, including elementary kinetics, evolution of solid phases as well as mass and charge transport. Implemented reaction mechanisms include a global model, a semi-elementary model according to Kumaresan et al. [2] as well as a more detailed model with surface states and a total of almost 20 elementary reaction steps. The charge and discharge processes involve the dissolution and precipitation as well as the chemical transformation of phases in the cell's electrodes [3]. The model is implemented in the in-house software DENIS [4].

We present simulated charge and discharge curves, concentration profiles and electrochemical impedance spectra. A typical discharge curve with phase behavior is shown in Fig. 1. The model is used to increase our understanding of the Li/S cell.

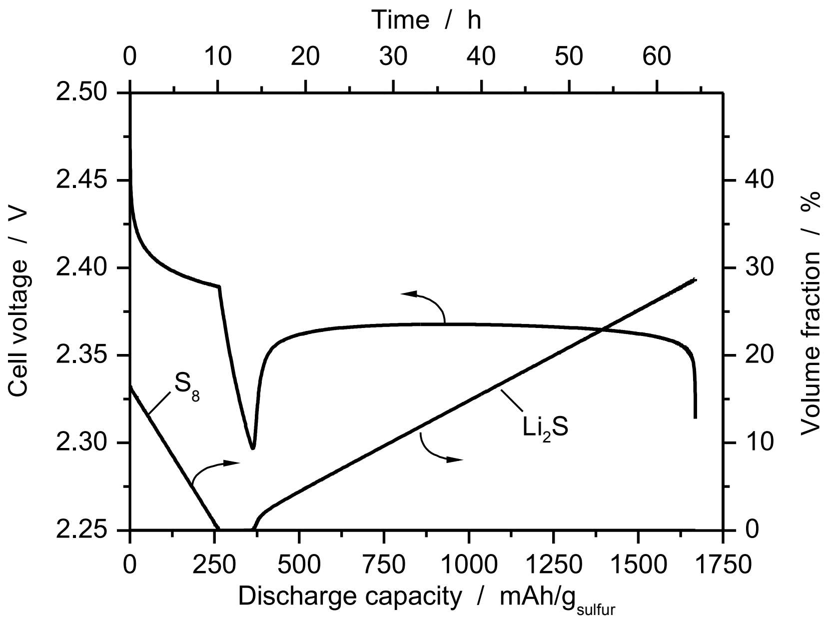

Figure 1: Simulated discharge profile of a Li/S battery with cell voltage (left axis) and volume fractions of sulfur (S_8) and Li_2S in the cathode (right axis).

References:

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