Influence of electrolyte and cell design on the performance of a Li-air button cell: a multi-step kinetics and 2D transport model

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A better understanding of the (electro-)chemical reaction mechanisms responsible for the formation and dissolution of the discharge products in Li-air cell is needed to improve the cell discharge capacity, cycling efficiency, and charging overpotential [1]. Here, a multi-methodology approach is applied to investigate the effect of underlying multiscale physico-chemical phenomena on the performance of a Li-air cell.

Firstly, with the help of a one-dimensional detailed-chemistry model [2], we investigate different multi-step reaction mechanisms for the formation of lithium peroxide (Li_2O_2) in the electrolyte bulk (solution mechanism), and alternatively, the formation of Li_2O_2 via an intermediate reaction step involving lithium superoxide (LiO_2) formation on the electrode surface (surface mechanism). Galvanostatic discharge and charge simulations are compared to experimental data and the crystal growth of the LiO_2 and Li_2O_2 are quantified.

Secondly, with the help of a two-dimensional (2D) axi-symmetric model [3], we investigate the influence of species transport and cathode geometry on the performance of a Li-air button cell. By focusing on the 2D distribution of species concentrations and porosity change (due to Li_2O_2 precipitation), we evaluate cell performance under different cathode thicknesses [4]. Furthermore, a detailed discussion on local current density distribution and electrode volume utilization is presented to understand the design induced performance limitations.

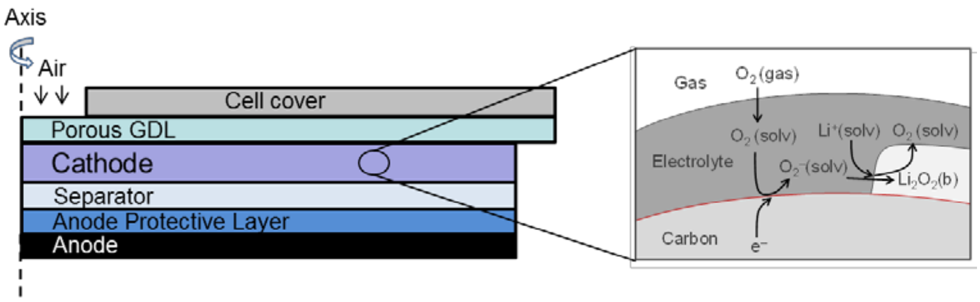

Fig 1: Schematic of the 2D axi-symmetric Li-air cell model and a zomed perspective of the reaction interfaces.

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