



Analysis of electrolyte level change in a lithium air battery

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H I G H L I G H T S

- A 2D Li-air coin cell model that can track electrolyte level change is developed.
- Results show that neglect of electrolyte level change underestimates cell capacity.
- The final distribution of the Li_2O_2 shows a peak in the middle of the cathode.
- Size of air chamber has significant effect on cells using volatile electrolyte.

A R T I C L E I N F O

Article history:

Received 19 August 2015
Received in revised form
16 December 2015
Accepted 18 December 2015
Available online xxx

Keywords:

Lithium air battery
Deformed mesh
Modeling
Electrolyte level

A B S T R A C T

A two-dimensional physical model that employs the deformed mesh method to track the electrolyte level in a Li-air coin cell battery is presented and used to investigate the effects of electrolyte level drop during cell discharge. The electrolyte level drop is caused by solid phase volume decrease and electrolyte solvent evaporation. Simulation results show that by neglecting the drop in electrolyte level, a Li-air battery model would under-estimate cell discharge capacity by as much as 22.5% in the parameter range studied. This counter-intuitive result is explained by an in-depth analysis of simulation results. A more realistic prediction of Li_2O_2 deposit distribution is obtained, with the peak value of Li_2O_2 volume fraction in the middle of the cathode instead of on the top surface, as predicted by previous studies. The interaction between the battery and its surroundings is considered by incorporating the air chamber into the computation domain. The diffusion of solvent vapor and oxygen in this chamber is included. For batteries using volatile solvents such as DMF, increasing the air chamber radius from 5 cm to 15 cm would result in a 72% increase of discharge capacity at the cost of losing a large amount of electrolyte.

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1. Introduction

Because of their high theoretical energy density, lithium air (Li-air) batteries, including lithium oxygen ($\text{Li}-\text{O}_2$) batteries, are considered to be promising candidates as the next generation secondary power supplies for portable devices and electric vehicles. A number of continuum-scale models have been developed to study the detailed charge and mass transport processes inside a Li-air battery. The first reported simulation model for Li-air batteries was by Sandhu et al., in 2007 [1]. Since then, various research groups have incorporated additional details to build more comprehensive models. Albertus et al. [2] was the first to consider solid product precipitation. Wang and Cho [3] developed a model to consider the coverage of reaction surface for different electrode

pore shapes. The model by Sahapatombut et al. [4,5] was the first reported to include the charging process and side reactions. Li and Faghri [6] developed a 2-D model and found that the micro pores closer to the separator/cathode interface were not fully utilized. They proposed a gradient cathode structure to increase specific capacity. Several models [7–9] considered the size distribution function of the pores or carbon particles in the cathode.

All previous studies neglected two important physical phenomena in a Li-air cell. The first is the electrolyte level drop during discharge caused by a decrease in solid phase volume. During discharge, the metallic lithium of the anode is converted to lithium ions, enters the electrolyte and moves to the cathode. In the micro-pores of the cathode, oxygen reduction reaction (ORR) occurs and consumes the lithium ions and electrons. Experimental studies [10] prove that insoluble and partially insulating Li_2O_2 is the major product of this reaction in non-aqueous electrolyte; therefore the overall reaction can be expressed as:

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According to the above equation, for each mole of lithium consumed 0.5 mol of Li_2O_2 are generated, which translates to 13.0 cm^3 of solid consumed and 9.93 cm^3 of solid generated. This means a 23.6% decrease of solid phase volume for each unit volume of lithium anode consumed during discharge. This vacated space must be replaced by the liquid electrolyte and therefore electrolyte level drops during discharge.

Fig. 1 shows the structure of a typical Li–air coin cell used in previous experimental studies [11,12]. The cell is normally placed on a solid surface with breathing holes facing upward, exposed to an air chamber. To compensate for the volume change, a spring is placed under the anode current collector in the cell. This ensures a tight contact between anode, separator, cathode, and current collectors in the cell. Solid volume decreases during discharge and electrolyte level drops. This effect is noted as an unsolved issue by Yuan et al. [13]. Yoo et al. [14] attempted to address this problem through a 1D model. However, the proposed model assumed a fixed anode and the battery is placed vertically.

The solid phase volume change is not the only factor to cause electrolyte level change. The evaporation of solvent is another phenomenon that is often neglected in modeling works. Most experimental studies on non-aqueous Li–air batteries used volatile solvents such as 1,2–dimethoxyethane (DME) and acetonitril (ACN), as indicated by Balaish et al. [15], to achieve a high oxygen solubility and diffusivity. Evaporated solvent escapes the battery through the breathing openings and is lost in ambient air. To our best knowledge, no previous modeling studies of the effect of solvent evaporation on cell performance have been reported.

Another often neglected physical phenomenon in Li–air battery models is the interaction of the cell with its surroundings. Lithium air batteries normally interact with their surroundings by consuming or releasing oxygen during the discharge and charge cycles, respectively. However, the computation domain of most existing Li-air battery models is generally bound by the interface of the cathode and ambient air, and assumes a constant dissolved oxygen concentration as the boundary condition. The diffusion of oxygen from the environment into the cell and solvent diffusion

into the environment have not been considered in prior studies.

In this paper, the previously neglected physical phenomena are included in our proposed two dimensional transient Li–air coin cell model. These effects on cell performance are examined and discussed based on simulated results. The Arbitrary Lagrangian–Eulerian (ALE) method is employed to describe the deformed computation domain and to track the moving electrolyte level. The air chamber that provides oxygen to the cell is included in the computation domain. The simulation results, both with and without consideration of these effects, are compared and discussed.

2. Physical model

The battery to be modeled has a typical coin cell structure, as shown in Fig. 1, and has been widely used in previous experimental studies. Structural parameters of the cell are listed in Table 1. The thickness of the cathode is $800 \mu\text{m}$. This value is chosen based on two reasons. First, using a thin cathode means higher percentage of the battery volume is occupied by separator and gas channel, consequently leads to a lower overall capacity. To achieve a competitive capacity, a thicker cathode must be used. Secondly, in most experimental and simulation studies, the cathode thickness is in the range between $500 \mu\text{m}$ and 1 mm [4–6,16,17]. It is assumed that the gas diffusion layer (GDL), cathode, separator and anode lithium metal have the same radius. To reduce the model to two dimensions, a single breathing hole is located at the center of the cathode casing. An axisymmetric assumption is adopted and the total computation domain is shown by the grey area in Fig. 2, which contains five sub–domains: the air chamber, GDL, cathode, separator, and anode. The governing equations developed below are used on one or several sub-domains depending on the physical phenomena.

The following assumptions are included to make the computation feasible:

1. Li_2O_2 is considered completely insoluble in electrolyte and precipitates on the cathode pore surface immediately upon generation.

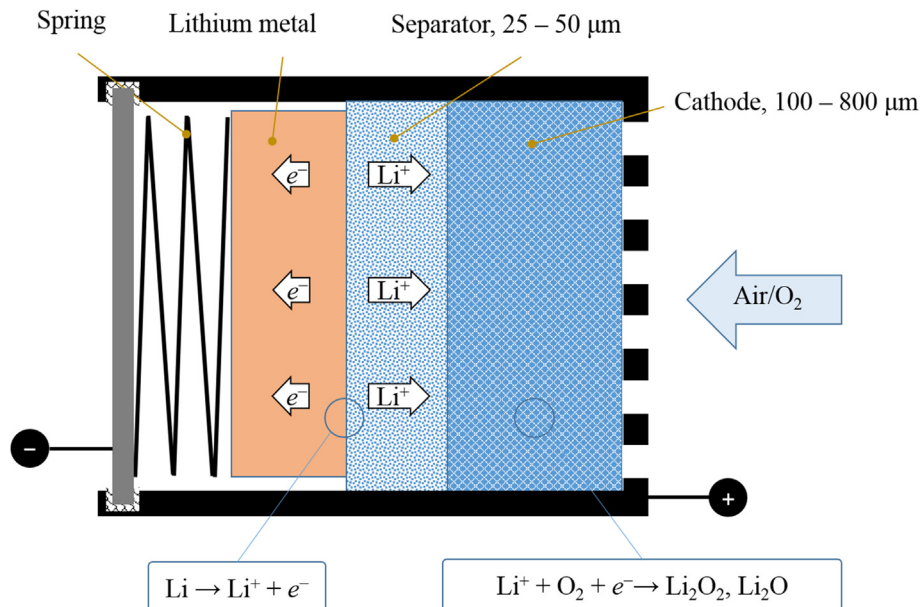


Fig. 1. Structure of a Li-air coin cell.

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