MODELING AND ANALYSIS OF A FLEXIBLE PAPER-BASED LITHIUM ION BATTERY

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Summary. The thermal analysis of the flexible paper-based lithium ion battery in different formations have been conducted using a two dimensional molecular dynamic model based on the Gibbs energy and Fick’s second law in COMSOL Multiphysics. The thermal analysis of the battery has been conducted in both charge and discharged cycles, using different packaging materials.

1 INTRODUCTION

The paper-based lithium ion batteries, is an answer for the need of having a durable and high power sources for flexible electronic devices. By combination of the paper-based and lithium ion materials, these batteries can provide high capacity/cyclability and flexibility. The fabricated batteries are using conventional lithium ion active materials over the highly conductive paper-based current collectors inside a polymer pouch packaging. The formation of the nanomaterials over the paper fibers changes some characteristics of the paper such as thermal and electrical conductivity ¹. Thermal management of the paper-based batteries, plays a big role in the performance of the lithium ion cells. The basic model for heat in these batteries is based on the migration of lithium ions from cathode to anode in charge and vice versa in discharge cycles, and migration of electron from the outer circuit. This electrochemical reaction inside the cell generates reversible and irreversible heats per unit volume ²,³. The irreversible heat is based on the polarization of active materials in electrochemical reactions, while the irreversible one is based on the ohmic potential drop in the electrodes, and change of the entropy. The reversible heat is the main parameter that is needed during each cycle, while the irreversible heat is only significant in high C rates ²,⁴. The mathematical model is based on the Fick’s second law and it is based on the flux of lithium ions in the closed environment of the cell. In addition, the previously reported, one and two dimensional model are not providing
accurate results while the effect of the heat dissipation in the pouch and paper current collectors are not considered \(^4,5\). The modified model provides a better understanding about the thermal management of the designed batteries, throughout the different working conditions such as bending, and using different packaging materials.

2 THE COMSOL MULTIPHYSICS MODEL

The CAE software selected for this Electrochemistry simulation and analysis is COMSOL Multiphysics 5.3. In this simulation it is essential we include heat analysis and hence the use of multiple physics i.e. battery domain and heat transfer come into picture. In this case LiClO\(_4\) (LCO) material has been chosen over the paper-based substrate and flexible packaging. The strategy used here is first have a one-dimensional model consisting of the materials used only in the battery’ active domains, referring to it as a cell. Followed by this, we introduce a two-dimensional model consisting of the current collectors and the packaging material, which constitute as a wholesome battery. This is the approach that has been adopted based on the size and shape of the components.

3 SIMULATION RESULTS

Under this set of results, we obtain plots that shows the electrochemical and thermal analysis of the system. Figure 1a is plot shows the LCO electrode potential. Similar to the electrochemistry results, the generated heat has been reported in figure 1b. Here the simulation results are comparable with all the measured values from experiments. The working voltage plateau of the cell is 4.5 volts and the temperature is 300°K.

![Figure 1](image.png)

**Figure 1** a) Electrode potential of the simulated battery and b) Temperature in the active region of the battery. Inset) Temperature gradient inside the cell

REFERENCES