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Gabby Kogler  
Washington University in St. Louis

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Optimization Tactics of Lithium-Oxygen and Lithium-Carbon Dioxide Batteries to Increase Voltage Output

Gabby Kogler

Research Advisor: Xianglin Li

Washington University in St. Louis

I. Abstract

Lithium-ion batteries are important sources of renewable energy. The importance of lithium-ion batteries lies in their high energy density, reliability and sustainability. This makes them essential for modern life and the future of clean energy. Throughout this semester, the goal of my independent study was to determine means for the optimization of the lithium-ion battery through variable changes and testing. I facilitated the assembly and disassembly of the battery cells and was able to compile data to make observations about the performance of the battery cells. As such, I was able to determine oxygen as the optimal gas to flow through the cathode of the battery cell and a clear indication of the optimal direction of the microporous layer (MPL) facing the separator within the cell. As such, many other experiments were conducted to make observations about the performance of the batteries such as changing the electrolyte amount, MPL size and examining the hydrophilic nature of the gas diffusion layer (GDL) via application techniques. Overall, the independent study was successful in learning assembly and disassembly techniques and making predictions about the behavior of the cells. Additionally, experiments

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1 Undergraduate Student, Department of Mechanical Engineering, Washington University, St. Louis, MO 63130, USA

2 Xianglin Li Professor, Department of Mechanical Engineering, Washington University, St. Louis, MO 63130, USA
could be conducted to examine the effects of changing other factors on battery performance such as electrolyte concentration, external environments such as temperature and humidity, types of less hydrophobic MPL, sizes and shapes of the cathode flow channels, etc.

II. Introduction

In recent years, lithium-air batteries have emerged as a promising alternative to traditional lithium-ion batteries due to their high energy density and potential for long-range electric vehicles. Lithium-air batteries are electrochemical devices that use oxygen from the air as a cathode material, which results in a significantly higher energy density than conventional batteries [2]. The use of air as a cathode material also reduces the weight and volume of the battery, making it an ideal candidate for electric vehicles and other portable devices.

For the lithium-air and lithium-carbon dioxide batteries, a simple chemical reaction occurs that yields a high energy result. For the lithium-air battery, the reaction occurs between the solid lithium chip and the $O_2$ gas. The reaction can be denoted below [1]:

$$2Li^+ + O_2 + 2e^- = Li_2O_2$$

and the reaction for the lithium-carbon dioxide batteries can be denoted below:

$$4Li^+ + 3CO_2 + 4e^- = 2Li_2CO_3$$

As shown, the chemical reactions for the lithium batteries yield an output of electrons, which in turn are collected on the cathode of the battery cell, thus producing a specific charge capacity for the MPL and GDLs of the cell.

However, despite their potential, lithium-air batteries still face several challenges, including the instability of the electrolyte, low efficiency, and short cycle life. There is a need for further research and development to overcome these challenges and bring lithium-air batteries to commercialization [3].
This research paper aims to contextualize the research being conducted to optimize the voltage output of lithium-air batteries via variable changes. Over the course of the semester, I worked alongside PhD candidate Amirhossein Sarabandi implementing these strategies. We worked to understand ways in to change certain features such as electrolyte amount, MPL or GDL facing the airflow channels of the cathode, air versus carbon dioxide through the airflow channels, and size of MPL carbon cloth. A such, understanding how changing these features affects the specific charge and discharge capacity of the battery becomes important at a fundamental level. Additionally, repeating these experiments to underscore the validity of our results was an important part of our project.

III. Methods

The overall construction of the battery remained the same across all batteries. However, within the assembly of the battery, several factors were altered to take experimental data from changing variables within the battery cell.

The asymmetric cell was constructed within a glovebox. The glovebox provided an oxygen-free environment in which the lithium chips would be unable to react with the outside air. After being voided of any outside contaminants or moisture, the cathode and anode of the battery were placed inside the glovebox. In addition to the anode and cathode of the battery, CeTech carbon cloth was placed inside and cut to a specific size (either 5/8” or ½” diameter) depending on the size of the flow channel. 6 nuts and bolts were placed inside as well as well as a gasket cut to an appropriate size to seal the components of the battery. Figure 1 below shows the battery in its disassembled form, showcasing the cathode and anode as well as the MPL facing the white separator.
Within the glovebox were items necessary for the construction of the battery. A solution of electrolyte with a 1:4 mass ratio between Lithium Bis(trifluoromethanesulfonic)imide (LiTFSI) and Dimethyl Sulfoxide (DMSO). This solution was obtained by measuring 5mL of the DMSO and obtaining the mass. Using the mass ratio, dividing the mass of the liquid by 4, the lithium salt powder was measured accordingly and added to form a homogenous solution as the electrolyte.

The battery was with either the GDL or MPL facing the cathode channel. A separator was placed on top of the carbon cloth and a lithium chip was placed in contact with the anode of the battery cell. As such, tests were conducted to observe the hydropic behavior of the MPL and its effect on voltage output. For one experiment, the assembly of the battery was the same for identical cells (i.e., same electrolyte amount, MPL size, etc.), except the assembly took place on the cathode as well as the anode. As such, the difference in assembly tested the difference in absorption for the GDL of the carbon cloth verses the MPL of the cloth.
Once the battery cells were constructed, the airways were sealed using parafilm such that when removed from the glovebox, no air could flow through the channels resulting in a premature reaction. The cells remained inside the glovebox overnight to complete the electrolyte absorption processes.

![Assembly of the battery cells with nuts and bolts.](image)

**Figure 2: Assembled cell with nuts and bolts.**

Once the cells were removed from the glovebox, they were hooked up to a Squidstat Plus to obtain data regarding the cells. Over the course of a few days, the voltage output was plotted against the current from discharging and charging the batteries. Once the batteries died as indicated by an instantaneous switch between charging and discharging, the batteries were disassembled.

**IV. Results**

In order to determine the efficacy of certain variable changes via the battery cells, plots were created showing the relationship between voltage and specific discharge capacities of the MPL within the cell. In order to find the specific discharge capacity of the cell, the following equation was used:

$$|Q_c \div A| - |Q_o \div A| \quad (3)$$
In eq. 1 $Q_C$ ($mA$) is the cumulative charge as recorded, $Q_o$ ($mA$) is the original cumulative charge, and $A$ is the working electrode mass-area ($mg/cm^2$). Based on this calculation, the specific charge and discharge capacity was recorded in $Ah/g$.

As such, the different graphs showing the relationship between voltage and specific discharge capacity yielded significant results. Battery cells were assembled and disassembled 3 times to determine the validity of results. Figure 3 below shows the relationship between voltage and specific discharge capacity for $0_2$ through the flow channels of the battery cell for $120 \mu L$ and $160 \mu L$ of electrode applied to the MPL.

![Graph showing the relationship between voltage (V) and specific discharge capacity (Ah/g) for 120 \mu L and 160 \mu L with 0_2](image)

As shown in Fig. 3, three trials were conducted for each of the electrolyte amounts. The $160 \mu L$ 2nd experiment yielded the highest discharge capacity. However, as indicated by the graph, the results weren’t consistent. As such, due to the inconsistency, there was no way to definitively provide a relationship between the efficacy of a battery and the electrolyte amount placed on the MPL.
Similarly, experiments were conducted by observing battery cell response to $C0_2$ instead of $O_2$. Figure 4 below shows a graph showing the relationship between voltage and specific discharge capacity for the lithium-$O_2$ and lithium-$C0_2$ battery cells.

![Graph showing the relationship between voltage (V) and specific discharge capacity (Ah/g) for 160 $\mu$L with $O_2$ and $C0_2$.](image)

**Figure 4: Graph showing the relationship between voltage (V) and specific discharge capacity (Ah/g) for 160 $\mu$L with $O_2$ and $C0_2$.**

As shown in fig. 4, the $O_2$ and the $C0_2$ experiments yielded different results in terms of specific discharge; however, from the graph we can discern less fluctuation in values of voltage for the $O_2$ experiments. This indicates $O_2$ as a more viable source to catalyze the internal reaction within the battery cell. This would make sense given the limitations surrounding carbon dioxide for lithium-ion batteries. One of the main issues that $C0_2$ provides is the reduction reaction rate of the discharged product Li$_2$CO$_3$ is very slow. These carbonates can reduce the battery’s capacity and cycle life. This can be observed in Figs. 5 and 6 below.
Figures 5 and 6 indicate the specific discharge capacities between two cells identically assembled. The difference between the two is indicated by oxygen versus carbon dioxide flowing through the channels of the cell. As shown visually by the graphs, the $O_2$ exhibit consistent voltage readings for all cycles given the shape of the curves. Additionally, there is less
significant drop off between the cycles compared to the carbon dioxide cycles. For the carbon
dioxide battery, the maximum specific discharge capacity goes from just over 0.625 Ah/g to 0.01
Ah/g in four cycles whereas for the oxygen battery, the capacity degrades less significantly from
0.512 Ah/g to 0.02 Ah/g in the four cycles.

An additional test was conducted to observe the performance of the battery based on the
orientation of the MPL. As shown by Fig. 7 below, it was determined that the MPL would be
most effective facing the separator within the battery. As such, the results below indicate this
observation.

![Graph showing the relationship between voltage (V) and specific discharge capacity (Ah/g) for 120 μL for O₂ for four discharge cycles with MPL facing the channels of the cathode](image)

As shown in Fig. 7, the specific discharge capacity was nominal even on the first cycle.
Whereas the batteries with the MPL facing the separator exhibited initial discharge capacities of
upwards of 0.5 Ah/g, the first cycle of the battery yielded slightly more than 0.004 Ah/g and was
essentially depleted after only three cycles. The main function of the MPL is to facilitate the
transport of oxygen from the air to the cathode while preventing the flooding of the cathode with electrolyte. As such it would make sense that placing the MPL facing the separator is crucial for the proper function of the battery to ensure long-term stability and performance

V. Conclusions and Future Work

Via numerous tests and experimentation, several relationships were found, but not proven by changing variables that would enhance or impede the performance of lithium batteries. For one, oxygen was found to have the best effect on battery performance as opposed to carbon dioxide. Additionally, the orientation of the MPL had a great effect on the battery performance – the MPL must face the separator to obtain charge and discharge capacity. While many relationships were not able to be proven via experimentation, further tests could be conducted in order to determine the relationship between electrolyte amount and battery output. As such, in the future, the research done for this project could be carried over for the further optimization of the battery cell. It would be useful to test certain electrolyte concentrations, more hydrophilic MPLs for better absorbance of the electrolyte and other sizes of cathode flow channels.

The research being conducted in this lab holds implications within the field of renewable energy. As researchers aim to find renewable energy sources as fossil fuels deplete and global warming exists as a prevalent issue, ways to optimize lithium-air batteries becomes more and more important. The batteries created within the lab could be implemented into technology, transportation, medical devices and many other industries.
VI. References

