Lithium Batteries: Structure and Efficiency
Optimizing Charge Time

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Abstract

The placement pattern of particles inside the anode of lithium ion batteries is known to affect the charge time of these batteries. The task of this research was to design a model that can check every possible configuration of particles and accurately predict the configurations of shortest charge time. Python was used to write the code for the model. Using the UI Campus Cluster, this model checked every possible configuration, excluding symmetry.

1 Theory and Motivation

Figure 1: A diagram of the charging process of lithium ion batteries. Azriel, Merryl. Dreamliner Battery Woes Have ISS Implications Space Safety Magazine, January 18, 2013.
In order to charge a lithium ion battery, a power supply must be attached to the positive and negative leads of the battery. This power supply drives electrons out of the Cathode and into the Anode. This process leaves positively charged lithium ions in the cathode. These ions migrate to the electron dense anode where they will be drawn to the tin particles. Governed by the Butler-Volmer equation, the lithium ions are then absorbed into the tin particles. The Butler-Volmer equation determines the ion current through the interface of a particle as a function of the potential difference across the interface and the number of ions involved. The placement of the tin particles in the anode affects how quickly the battery will charge. This is the motivation for this research. The aim of this project is to create a model which determines realistic trends in how particle patterns correspond to charge time.

2 Method

The Python code was written to model any desired configuration of particles. First, a grid size must be chosen. The most common choices for this research were $5 \times 5$, $10 \times 10$ and $20 \times 20$. A particle density must also be selected. A density of 0.5 was most often selected. This density corresponds to half of the cells being filled with particles and the other half being filled with electrolytes. This is represented in the code by an $N \times N$ matrix of ones and zeros. The ones represent the particles and the zeros represent the electrolytes. The charging process is carried out in iterations. Each iteration causes lithium to transfer from each cell (particle or electrolyte) to all of the eight neighboring cells. A different transfer rate was set for buffer-to-buffer, electrolyte-to-electrolyte, buffer-to-electrolyte and electrolyte-to-buffer transfers. Each cell was given an initial ion concentration of lithium. Above the top row of the grid is an infinite source of lithium.
lithium ions which diffuse into the grid during each iteration. Therefore, the
top of the grid tends to become dense with lithium ions before the bottom.
After each iteration, the concentration of each cell is updated. The starting
concentration of the cells is 1 for electrolytes and 0 for buffers. A fully charged
particle will have a concentration of 100. These are in units of approximately
1.3 nanomoles. Once the net capacity of all the particles is at least 95% full,
the battery is considered charged and the number of iterations in this process
is recorded. Constant voltage was assumed in this model. This means that
the power supply used to charge the battery is assumed to be operating at a
constant voltage. This assumption linearizes the Butler-Volmer equation which
will come in handy for future models of this research.

3 Results

![Figure 3](image)

Figure 3: On the left is one of the fastest charging configuration for a 5 × 5
grid. On the right is one of the slowest charging configuration. The red squares
represent buffers.

A text file of 1-0 strings was used to generate every possible pattern on a
5 × 5 grid. Using C, redundant patterns were removed. The grid is mapped onto
a cylinder, so lithium can transfer from one vertical wall of the graph to the
other. The patterns which were the same as others with shifted columns were
removed. Patterns which had horizontal rows were also removed since these
would never charge. The remaining patterns were run through the Python code
on the UI Campus Cluster for 12 days. Three patterns tied for fastest charge
time. It took 1097 iterations to bring them to a 95% charge. These patterns
all had the same trend of buffers arranged in columns. One of these patterns
is shown in figure 3. Over ten patterns tied for slowest charge time. It took
them 1500 iterations to reach only 43% charged. They all followed the trend of
having the upper triangle of the grid filled with buffers and the lower triangle
of the grid filled with electrolytes. One of these patterns is pictured in figure 3.

Pictured in figure 4 is a histogram which was generated from the data re-
ceived by the Campus Cluster. Approximately two million different patterns
were tested on the Campus Cluster and this histogram shows the distribution of how much charge the various patterns acquired. Notice that very few of them reached 95% after 1500 iterations.

Figure 4: The distribution of how much charge the patterns acquired after 1500 iterations. This includes every possible configuration on a $5 \times 5$ grid, excluding symmetry.

4 Future Work

The future of this project lies in making the model more realistic and using more sophisticated code to check the possible patterns. The model currently uses simple diffusion to describe how lithium travels through the cells. The future model will take into account the linearized Butler-Volmer equation at the interface of each particle under the assumption of constant voltage. As shown in figure 5, the future model will have $4 \times 4$ particles. The inner four squares hold the lithium. These inner squares are the only ones used for determining how much charge the battery has received. The outer layer of squares represents the interface of the particle. The transfer rate between outer and inner squares will
Figure 5: An idea for a more realistic particle including an interface.

be governed by the linearized Butler-Volmer equation. This more sophisticated version of the particles will hopefully provide more realistic trends in the charge times of various patterns.