Development and Analysis of Solid-State Batteries through Implementation of the COMSOL® Platform

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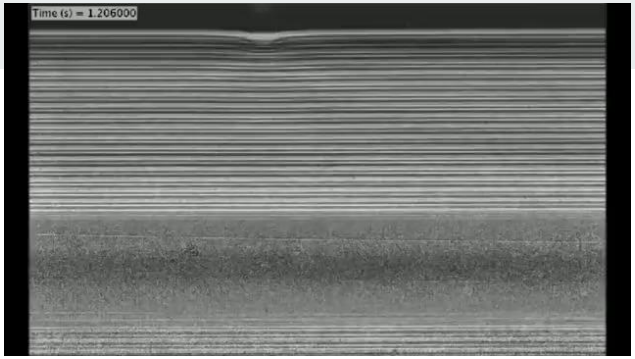


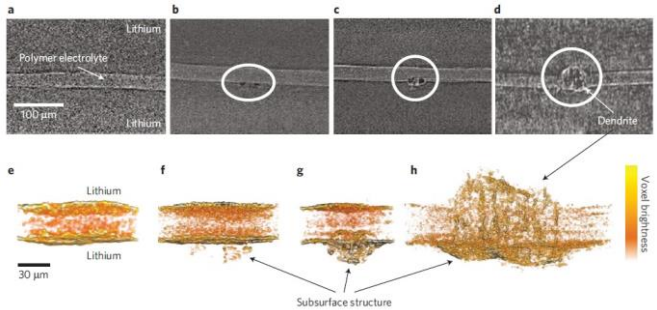
The Need for Solid-State

Energy density in liquid Lithium-Ion batteries has begun to plateau. Production of Lithium-ion batteries does not match the demands of consumers, industry, or development. We have grown accustomed to smaller and smaller devices, but each new iteration demands higher performance - the means of supplying power has to change for this trend to continue. Safe, efficient, and effective is great, but safer, more efficient, and more effective is better.

Solid-state batteries are:

- Less flammable
- More durable
- Longer lasting
- Kinder to the environment

  (in comparison to batteries with liquid lithium-ion electrolyte



Solid-State to Date

Solid-state battery research has been going on since the 1800s, but meaningful advances have been made in the last few decades towards the realization of such devices. Universities, industry leaders, and even the Department of Energy are moving towards fabricating and implementing solid-state batteries.

Within the last year alone, approximately $1.3 billion dollars have been dedicated toward energy storage research, with an estimated third of that wholly towards solid-state battery development. Start-ups developed solely around solid-state research are finding themselves with between $20 and $125 million for their efforts.

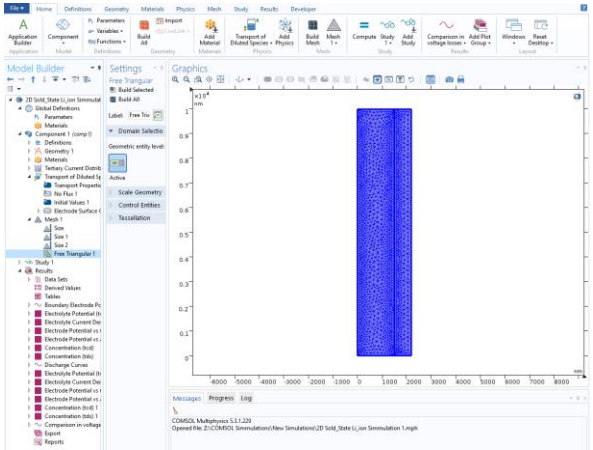
Benefit of Research with COMSOL®

COMSOL® lends itself to this research because of its flexibility and ease of use. We are able to modify geometries, equations, and more. COMSOL® allows us to add in multiple studies to gain the data needed.

For undergraduate students at a very small university, access to resources is limited. Using COMSOL® allows for the simulation of ideas and the ability to support claims before requesting lab time with professors.

An additional impetus for our research has been to pursue green initiatives. SSBs offer an efficient, therefore greener, alternative energy storage option, but COMSOL® provides an ecologically friendly means to conduct the research itself.

Solid State Battery Design and Simulation



2D Model Lithium Ion SSB

A 2D model was implemented so that the lithium ion transfer across the battery can be observed.

Battery Components and materials:

Positive Electrode Material: LiCoO2 Lithium Cobalt Oxide

Electrolyte Material Composition: Li3PO4 Lithium Phosphate

***The Negative Electrode is a lithium foil assumed to be an infinite source of Li-ions .*

Solid State Battery Design and Simulation

Batteries and Fuel Cells Module

Physics used:

Tertiary Current Distribution Interface
To model the electrochemical reactions.

Transport of Diluted Species Interface
To model the transport of lithium ions in the positive electrons.

The reaction kinetics in the study is described by the Butler-Volmer Equation. Fig3.

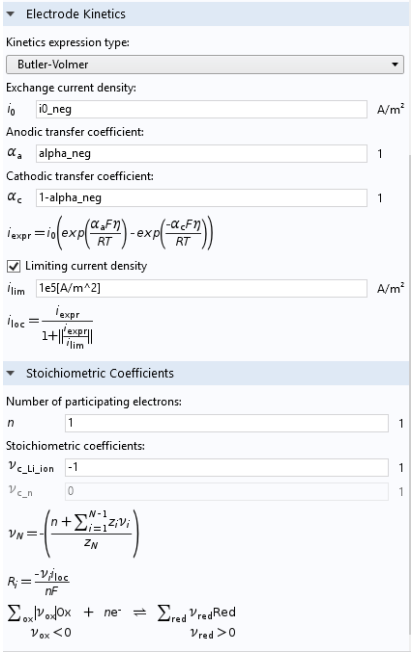


Fig3. Electrode reaction equations

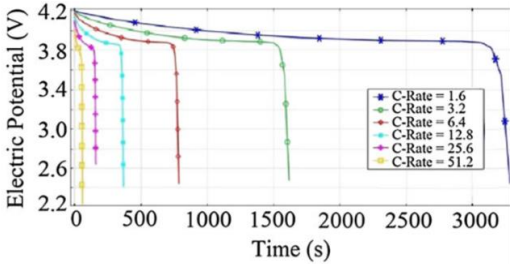
Variable	Value
$c0_{Li}^+$ [mol/m^3]	$6.01e^4$
Kr [m^3/(mol*s)]	$0.9e^{-8}$
δ	0.18
D_{Li}^+ [m^2/s]	$0.9e^{-15}$
D_n [m^2/s]	$5.1e^{-15}$
$c_{Li\text{-}max}$ [mol/m^3]	$2.33e^4$
D_{Li} [m^2/s]	$1.76e^{-15}$
α_{pos}	0.6
k_{pos} [mol/m^2/s]	$5.1e^{-4}$
T [K]	298.15
i_{1C} [A/cm^2]	10e − 6
α_{neg}	0.5
k_{neg} [mol/m^2/s]	1×10^{-2}

Fig4. The SSB model was implemented using the operating parameters found in the COMSOL® library

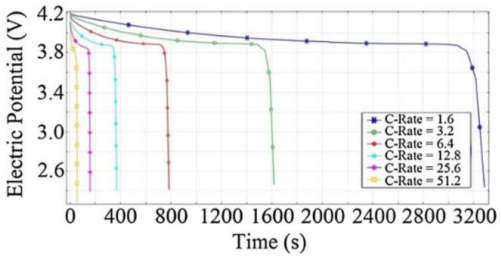
Solid-State Battery Design and Simulation

Our Goal:
The goal of this study was to compare the voltage drop across different sized geometries on each of the battery cells when specific C-Rates were applied. When the maximum activity value is reached the voltage curve will reach zero, signalling that the electrode can no longer contain more ions.

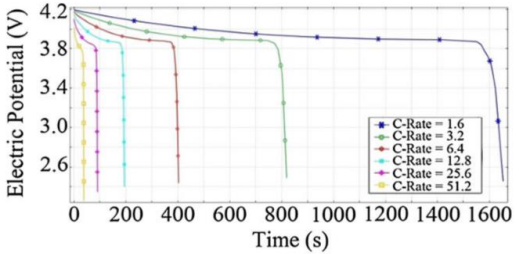
To evaluate the effect of varying operating geometric sizes, three cases were simulated.



1500nm-500nm



900nm-700nm



1500nm-700nm

Solid State Battery Simulation Results

- Time-dependent simulations of a 2D model with increasing C-rates were successfully performed. These simulations considered the electrochemical reaction and diffusion of Li-ions and electrons in the electrolyte and solid Lithium ion the positive electrode. The results shown provide important information about the behavior of the Li-ion SSB cell when discharged at different current densities.

Observations:

- The team noticed that with the smaller positive electrode thickness, the maximal ionic activity is reached much quicker resulting in a faster discharge curve with any C-rate. This happens because the positive electrode has reached the maximum level of solid lithium ions it can contain.
- Another observation is that when the electrolyte width was decreased, the lithium ions travel faster to the electrode, making the discharge curve complete its cycle at 1600 seconds at a C-Rate of 1.6.

What This Tells Us

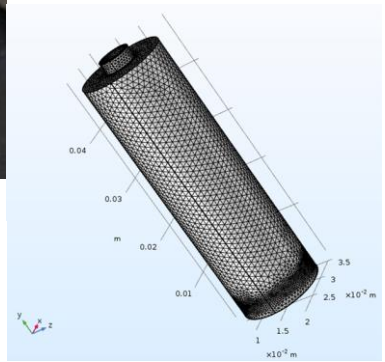
- A smaller electrode to electrolyte ratio means faster ionic transfer
  - Minimize the ratio without losing functionality
  - Verify findings in 3D
  - Delve into material options
  - Thin film and doping techniques
- Context for findings is needed
  - Numerical comparison to standard lithium ion
  - Effective meaning of discharge time in terms of battery usage

Future Research

- Materials testing
  - Graphene
  - Glass
  - Magnesium
- Fabrication
  - Requires 3D design and testing
- Implementation
  - Simulation testing

Image courtesy of www.canadianbusiness.com

Image courtesy of www.scurion.ch



Questions?