Ongoing Alternative Energy Storage Research and Development for Solid-State Batteries

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I. BACKGROUND

Over the years, the increase of energy density in lithium-ion batteries has begun to plateau. The impact of mainstream consumer electronics alone has doubled lithium-ion battery production, making it clear that the need for more viable energy storage solutions is immediate.² As technology advances, creating eco-friendly methods of transportation and combating the present state of climate change become priorities in development. The need to investigate new methods of storing energy and to improve standard battery chemistries is imperative to fully take advantage of new other sustainable technologies.

The trend towards solid-state battery technology is driven by efficiency on a variety of levels. Solid-state batteries have been proven to be a more eco-friendly alternative to their liquid counterparts.³ The use of solid electrolytes means batteries are both less flammable and more durable, since they are non-flammable and react much less frequently, hardly undergoing decomposition reactions, at all. This results in safer, more durable, longer lasting batteries. Maximizing the power density of solid-state batteries to match or surpass that of liquid lithium-ion batteries is integral to both the future of solid-state batteries as well as energy storage solutions and green energy practices.

Designing a system utilizing solid-state electrolytes sets the foundation for fabricating this kind of efficient, green, durable batteries. Extensive research in material science coupled with advances in computer databases have allowed researchers access to powerful software tools, such as the multi-physics numerical analysis platform, COMSOL©, that may be used for simulating the structural behavior before performing any lab experiments.

II. OBJECTIVE

The aim is to create an environmentally friendly and viable solid-state battery storage device with the combined efforts of utilizing finite element analysis software for designing the geometry and material selection. Simulation provides opportunities to explore different material properties and cell geometries to optimize a lithium-ion solid-state Battery performance.

Simulations are time dependent and must consider electrochemical reactions, the diffusion of lithium-ions and electrons in the electrolyte, and solid lithium diffusion in the positive electrode for a solid-state lithium-ion battery simulation. The Butler-Volmer equation would be used to examine the effects of the kinetic reactions of the lithium ions on the solid electrolyte and electrode interfaces ¹.

$$\begin{split} i_{\text{pos}} &= i_{0, \text{ pos}} (e^{(\alpha_{\text{pos}} F \eta) / (RT)} + e^{-((1 - \alpha_{\text{pos}}) F \eta) / (RT)}) \\ i_{0, \text{ pos}} &= F k_{\text{pos}} \left(\frac{(c_{\text{Li, max}} - c_{\text{Li, min}}) c_{\text{Li}}}{(c_{\text{Li, max}} - c_{\text{Li, min}}) c_{\text{Li}}} \right)^{\alpha_{\text{pos}}} \left(\frac{(c_{\text{Li}} - c_{\text{Li, min}})}{(c_{\text{Li, max}} - c_{\text{Li, min}})} \right)^{1 - \alpha_{\text{pos}}} \end{split}$$

$$i_{\rm neg} = F k_{\rm neg} \left(\frac{c_{\rm Li^+}}{c_{\rm Li^+}} \right)^{\alpha_{\rm neg}} \left(e^{(\alpha_{\rm neg} F \eta)/(RT)} + e^{-((1-\alpha_{\rm neg}) F \eta)/(RT)} \right)$$

The transport of positive lithium ions and negative charges is described by the Nernst-Planck equation:

$$\mathbf{N}_{i} = -D_{i}\nabla c_{i} + \frac{z_{i}F}{RT}Dc_{i}\nabla \phi_{1}$$

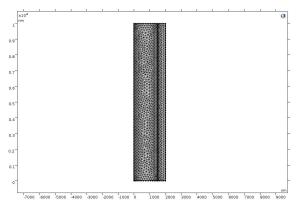


Figure 1. Geometric view of two-dimensional solid-state battery

III. CONCLUSION

Using a numerical analysis material reaction simulation software, a two-dimensional model of a lithium-ion solid-state battery could be created and used to generate accurate simulations of battery physics. Three two-dimensional solid-state batteries, each with electrodes of different sizes, were analyzed to compare the cell voltage and electrolyte ionic surface concentration in this project. The two-dimensional battery with larger electrode area reached its maximum activity value of solid lithium concentration at higher time compared to the smaller areas, suggesting that a solid-state battery with a smaller electrolyte layer compared to electrode layer may be best suited for future research, since the maximum activity value for solid lithium in the positive electrode is the maximum level of solid lithium the electrode is able to contain.

The next stage of this project is to perform laboratory evaluations of the materials and geometries simulated to fabricate a battery model to be tested and studied for similar attributes and characteristics. Ultimately, the aim is to construct a working battery module to serve as a storage unit for energy generated by green alternatives technologies such as solar and wind. While this long term goal serves to bolster green research and initiatives thanks to the ecologically friendly characteristics of solid-state batteries, the research, too, furthers this goal. The reliance on simulations to conduct preliminary investigations partnered with the focus on efficient technologies results in an overall environmentally conscious process.

Nomenclature

 i_{neg} = current density at negative electrode

 i_{pos} = current density at positive electrode

 \dot{k}_{neg} = charge transfer reaction rate constant at negative electrode

 $c_{i,+}$ = concentration of lithium-ion

 $c_{L,i+0}$ = initial concentration of lithium-ion

 α_{neg} = charge transfer coefficient at negative electrode

F = Faraday's constant

 η = overpotential

R = universal gas constant

T = temperature

 $i_{0,pos}$ = initial current density at positive electrode

 α_{pos} = charge transfer coefficient at positive electrode

 k_{pos} = charge transfer reaction rate constant at positive electrode

 $c_{\text{Li,max}}$ = maximal lithium activity in the positive electrode

 c_{Li} = solid lithium concentration

 $c_{\text{Li,min}}$ = minimum lithium concentration in the positive electrode

 ϕ_1 = electrolyte potential

 N_i = transport value of species i

 z_i = charge of species i

 D_i = diffusion coefficient for species i

 c_i = concentration of species i

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