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

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Abstract

This report explores the utilization of COMSOL® to investigate material properties and perform finite element analysis in solid-state batteries. 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 within recent years, making it clear that the need for more viable energy storage solutions is immediate. As technology advances, creating eco-friendly methods of transportation and combating the present state of climate change become priorities in development; battery technologies must adopt practices that progress towards this goal. 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.

Extensive research in material science coupled with advances in computer databases have allowed researchers and lab technicians access to powerful software tools that may be used for simulating the structural behaviour before performing any lab experiments. Through the use of a numerical composition simulation software, researchers are investigating materials, prototypes, and projects before implementing new solutions in the lab. This presents opportunities to make more informed decisions about materials to have in a project, spend less funds testing different substances, and gain valuable insight into the applications of these within solid-state batteries.

The COMSOL® platform provides the team with the ability to research underlying properties, such as, state of charge, charge capacity, and internal resistance, while also enabling more pointed material selection. Through its use, experimenters conduct theorized optimal adjustments using the various modules of COMSOL®, including: AC/DC, Semiconductor, Fluid Flow, Heat Transfer, Electrochemistry. These program components allow for the specification of behaviours and interactions for materials tested. This is integral in the pursuit of developing solid-state batteries that function efficiently, safely, and sustainably, since the specifications of such parameters will enable fabrication of energy storage solutions that are less detrimental to the environment, but have higher energy densities than Lithium-Ion batteries.

The first stage in developing such impactful technology is an in-depth finite element analysis of various prospective materials deemed to be possible components, as well as

arrangements of material combinations that maximize C-rate, resistivity, and capacitance. Through the use of the COMSOL® Electrochemistry module, specifically the Battery Interfaces subsection, the flow of electron transport within materials and simulated cells are monitored to investigate their impact on the structure's energy and power density. This enables the analysis of C-rate within prototypes and, using the AC/DC module's ability to utilize the designs in tandem with constructed electrical circuits and devices, implementation of the batteries and components generate pertinent information regarding its longevity. This is exemplative of the specifications to be refined within COMSOL® before the fabrication of real-world, testable, solid-state battery.

Figures used in the abstract

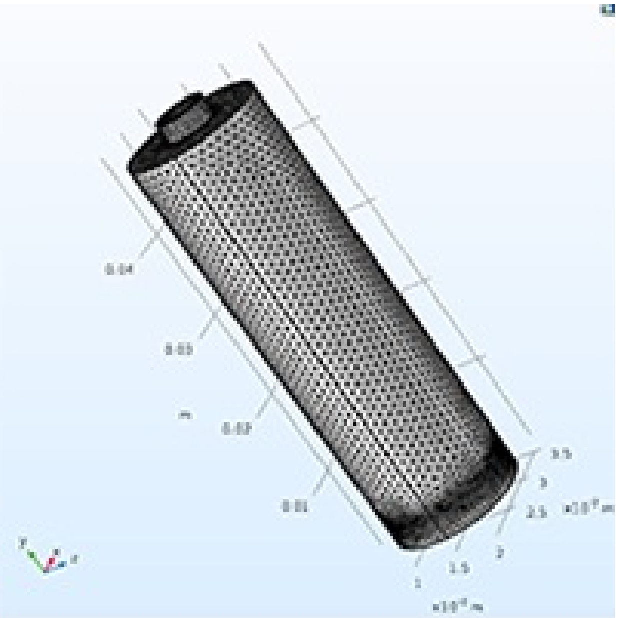

Figure 1: Using COMSOL® interface to generate an alkaline battery model