The Solid Mechanics of Solid-State Lithium-ion Batteries from Changing the Charge Rate and Elastic Modulus of the Electrolyte within the Cell

Gabby Kogler
Advised by Dr. Adam Boyce

Introduction

The increasing need for energy storage solutions has spurred demand for high-performance, long-lasting, and low-cost batteries, with solid-state batteries (ASSBs) emerging as a promising alternative to lithium-ion batteries due to their safety and potential for high energy density [1]. ASSBs operate through the movement of lithium ions between anode and cathode through a solid electrolyte, enhancing safety and energy density by eliminating leakage and volatility risks associated with liquid electrolytes [2]. The research in the project focuses on addressing ASSBs' limitations by understanding degradation mechanisms and mechanical stresses within the cell to improve performance, utilizing multi-physics models and stress analysis to optimize their longevity, efficiency, and safety.

Methodology

To investigate the solid mechanics of solid-state batteries, simulations were conducted using COMSOL Multiphysics software, enabling the modeling of battery cells under various conditions, including the full discharge and charge cycles in seconds, a process that takes significantly longer in experimental settings [3]. The software's Battery Design Module and the finite element method (FEM) were utilized to create detailed geometrical models of the batteries, facilitating the analysis of ion transport and electrical conductivity [4]. Parameters such as the charge and discharge rates and the elastic modulus of the electrolyte were systematically varied to assess their impact on the battery's solid mechanics. The stress on lithium particles was observed by altering the discharge C rates and the Young's modulus of the electrolyte, which influenced the battery's performance by indicating the stiffness or rigidity of the electrolyte and its resistance to deformation. The simulations were calibrated and validated against experimental data, ensuring the reliability of the models and contributing to the optimization of battery design and development of enhanced management strategies for solid-state lithium-ion batteries [5].

Results

To observe the solid mechanics of the particles, the cells underwent charge and discharge cycles, as shown in fig. 1. The cells with a lower C-rate achieved a closer discharge behavior to the equilibrium potential.

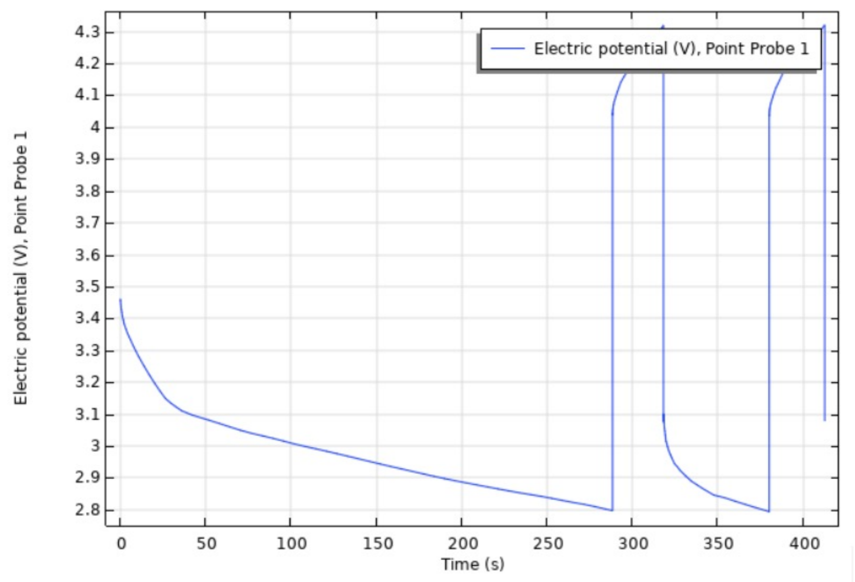

Figure 1: Prob plot (140 GPa, 3C)

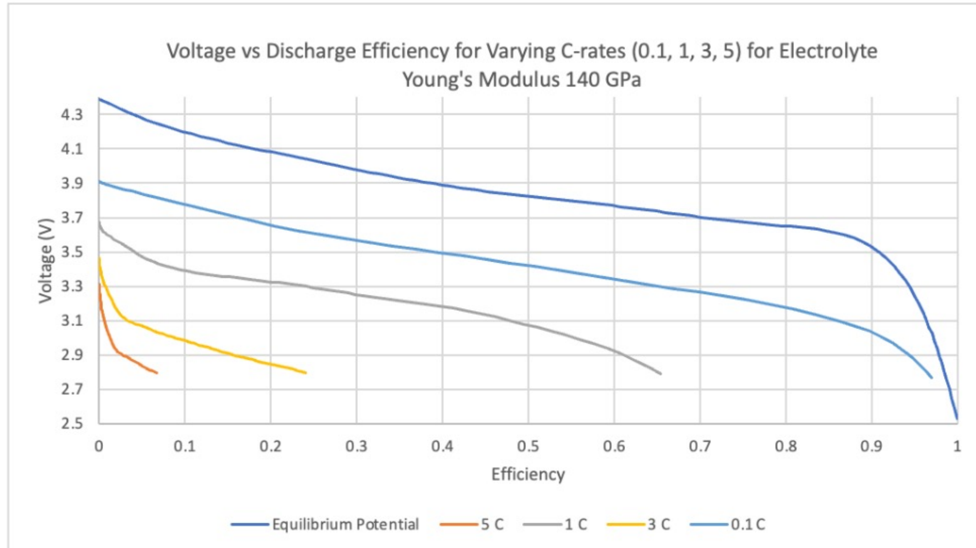

Figure 2: Graph showing the relationship between voltage and efficiency for varying C-rates with an electrolyte of Young's modulus 140 GPa

The lithiation and stress of the particles for the cells with 140 GPa elastic modulus for the electrolyte can be observed below. The images were captured at the end of discharge.

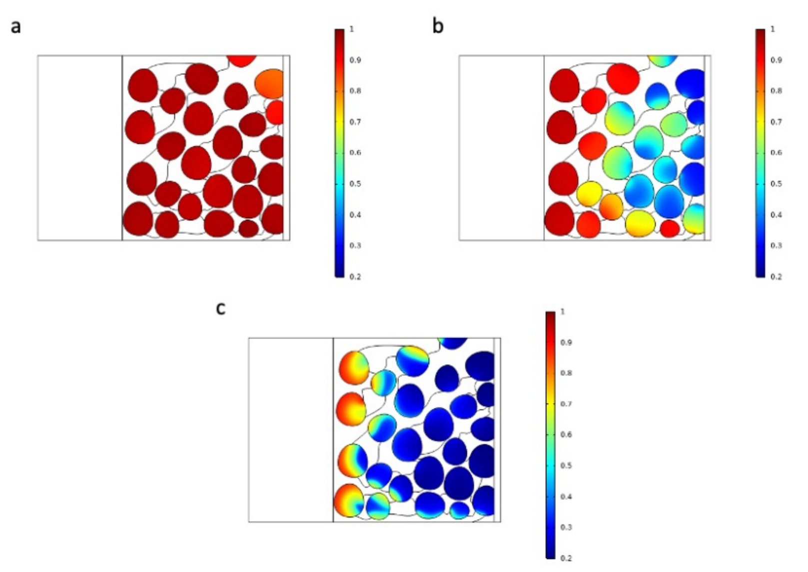

Figure 3: Lithiation profiles with electrolyte Young's modulus of 140 GPa with C rates of 0.1C (a), 1 C (b) and 3 C (c)

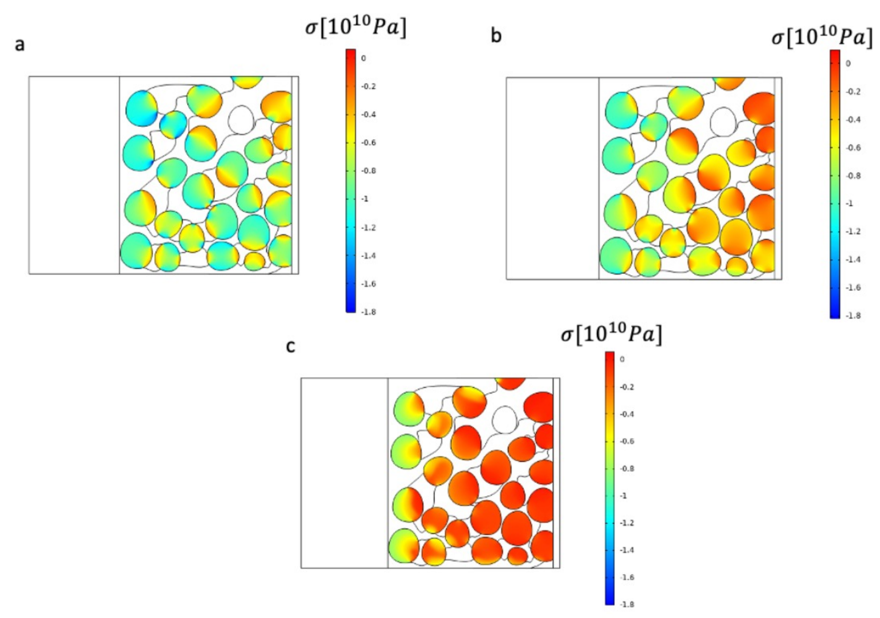

Figure 4: Particle stress with electrolyte Young's modulus of 140 GPa with C rates of 0.1C (a), 1 C (b) and 3 C (c)

To make comparisons about the effect of the elastic modulus of the electrolyte on the stress of the particles, the following images were generated. All models have equivalent C rates, but differing elastic moduli for the electrolyte.

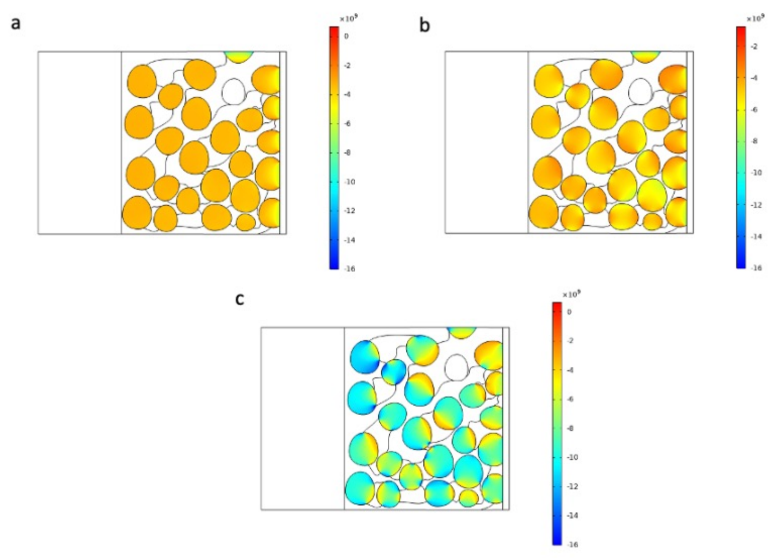

Figure 5: Particle stress with C-rate of 0.1 C with electrolyte Young's modulus of 1.4 Gpa (a), 14 GPa (b) and 140 GPa (c)

As means to draw relationships between altering the two variables, the two graphs were created below, observing how the peak stress for the particles as seen in fig.6 and the peak electrolyte stress as seen in fig. 7 are affected by altering the elastic moduli of the electrolyte and C-rate.

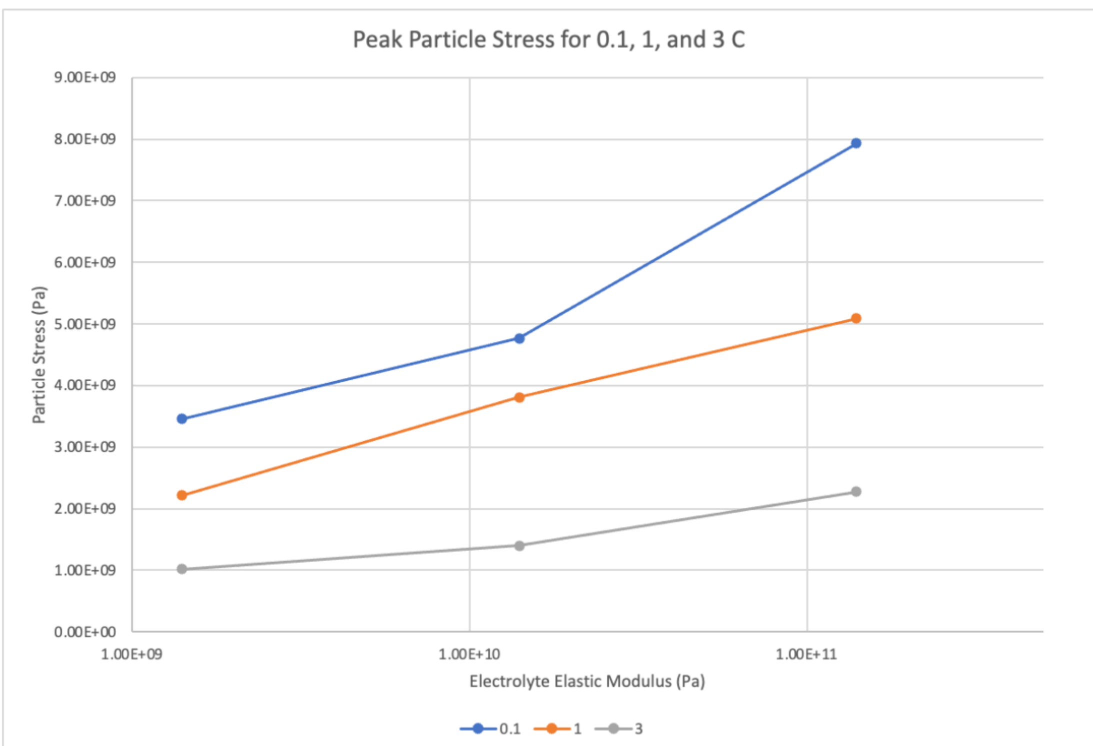

Figure 6: Peak particle stresses for different C-rates at different electrolyte elastic moduli

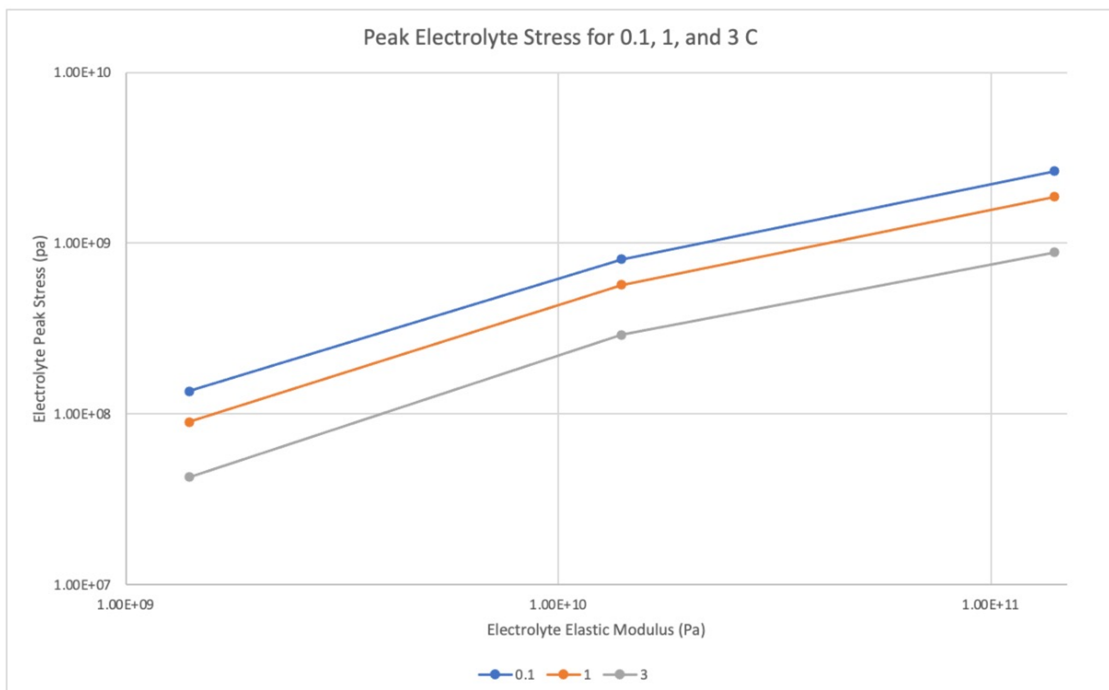

Figure 7: Peak electrolyte stresses for different C-rates at different electrolyte elastic moduli

Discussion

By observing the effects from changing the properties of the solid-state lithium-ion batteries, there is a better understanding of battery performance and ways to avoid degradation within the cells. As indicated above in the results section, increasing the C-rate leads to a gradient-like lithiation scale, and as indicated by the discharge graphs, a lower discharge capacity due to losses [7]. Additionally, the high stress concentrations, unevenly distributed from the higher charge rates indicates the battery's susceptibility to failure due to degradation of the cell. The elastic moduli of the electrolyte also plays a significant role in the solid mechanics of the particles. A higher elastic modulus of the electrolyte increases the stress on the particles when the they begin to swell. Being constricted by the rigid ceramic-like electrolyte, the stress of the particle would increase leading to failure due to cracking. As such, a critical relationship must be found between altering the two variables to ensure the lasting performance of the solid-state lithium-ion battery.

References: [1] M. Alabdali, F. M. Zanotto, V. Viallet, Vi. Seznec, A. Franco, "Microstructurally resolved modeling of all solid-state batteries: Latest progresses, opportunities, and challenges," Abbrev. Elsevier, vol. 36, 2022, doi: 10.1016/j.coelec.2022.101127. [2] J. Janek, W. Zeier, "Challenges in speeding up solid-statebattery development," Abbrev. Nature Journal, 11 January 2023, doi.org/10.1038/s41560-023-01208-9. [3] "BU-409: Charging Lithium-ion," Battery University, CADEX, 25 October 2021. [Online]. Available: https://batteryuniversity.com/article/bu-409-charging-lithium-ion. [Accessed: 22-Apr-2024]. [4] "The Finite Element Method (FEM)," COMSOL, Multiphysics Cyclopedia, 15 March 2016. [Online]. Available: https://www.comsol.com/multiphysics/finite-element-method. [Accessed: 22-Apr-2024]. [5] A. Sakuda, A. Hayashi & M. Tatsumisago, "Sulfide Solid Electrolyte with Favorable Mechanical Property for All-Solid-State Lithium Battery," Abbrev. Scientific Reports, vol. 3, no. 2261, 23 July 2013, doi: 10.1038/srep02261. [6] H. Yu , D. Taha, T. Thompson, N. Taylor, A. Drews, J. Sakamoto, K. Thornton, "Deformation and stresses in solid-state composite battery cathodes," Abbrev. Elsevier, vol. 440, 2019, doi: 10.1016/j.jpowsour.2019.227116.