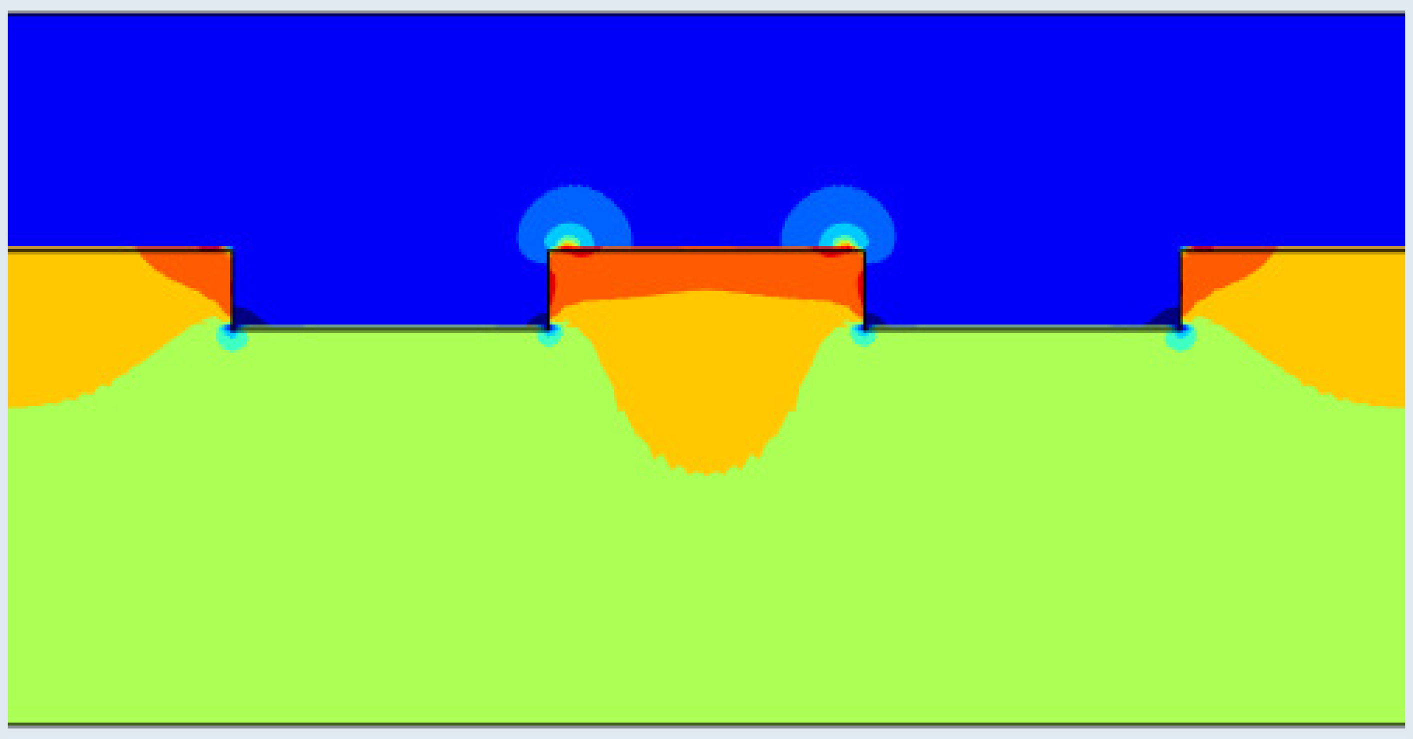

Evaluating Interfacial Evolution in Thin-Film All-Solid-State Lithium-Ion Battery via FEM Modeling

Enhance the practical implementation of All-solid-state lithium-ion batteries (ASSLIBs) through a comprehensive understanding of their behavior.

T. H. Gebregeorgis, J. R. Busacker, X. Zhu, A. Hubin, M. H. Mamme
Research Group Electrochemical and Surface Engineering (SURF), Department of Materials and Chemistry, Vrije Universiteit Brussel (VUB), Brussels, Belgium

Abstract

ASSLIBs have gained increasing attention as potential game-changers in energy-storage technology. These batteries offer improved safety, higher energy density, and longer lifespans. However, the development and commercialization of ASSLIBs are hindered by manufacturing difficulties [1] and a limited understanding of the process occurring at the solid electrolyte/electrode interface [2-4] due to the complexity of the battery system and the lack of experimental techniques to investigate these processes. The findings offer greater insight into the behavior of ASSLIBs, particularly by capturing the mechanical stress that occurs within ASSLIBs. This information serves as a useful resource for improving the design of ASSLIBs.

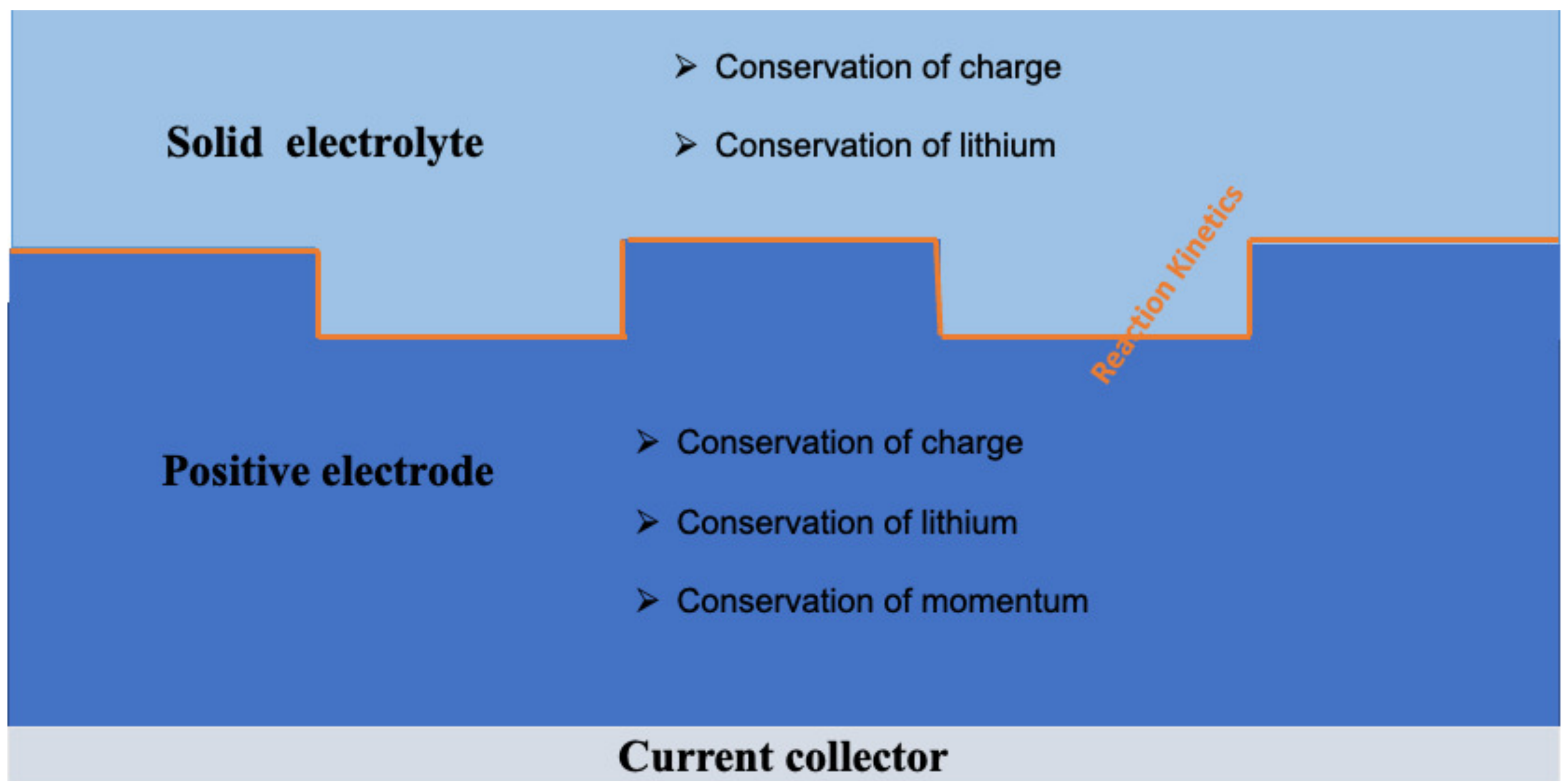

FIGURE 1: Model geometry

Modeling Approach

A fully coupled electro-chemo-mechanical ASSLIBs was modeled in 2D. Mechano-electrochemical processes occur when lithium ions diffuse from the cathode to the cathode/SE interface and are involved in oxidation reactions, with the generated Li ions traveling through the SE to the anode/SE interface, where they are reduced to Li. The Li is then travelled into the anode. The top and bottom border displacements are set to zero.

Results

The simulation results (Figure 2) revealed that the highest mechanical stress is found at/near the edges/corners of the patterned geometry, electrode/solid electrolyte interface, due to the sharp change in geometry indicating a higher risk of mechanical failure. This finding suggests that the mechanical performance of the patterned thin film structure is strongly influenced by the design of the electrode/solid electrolyte interface.

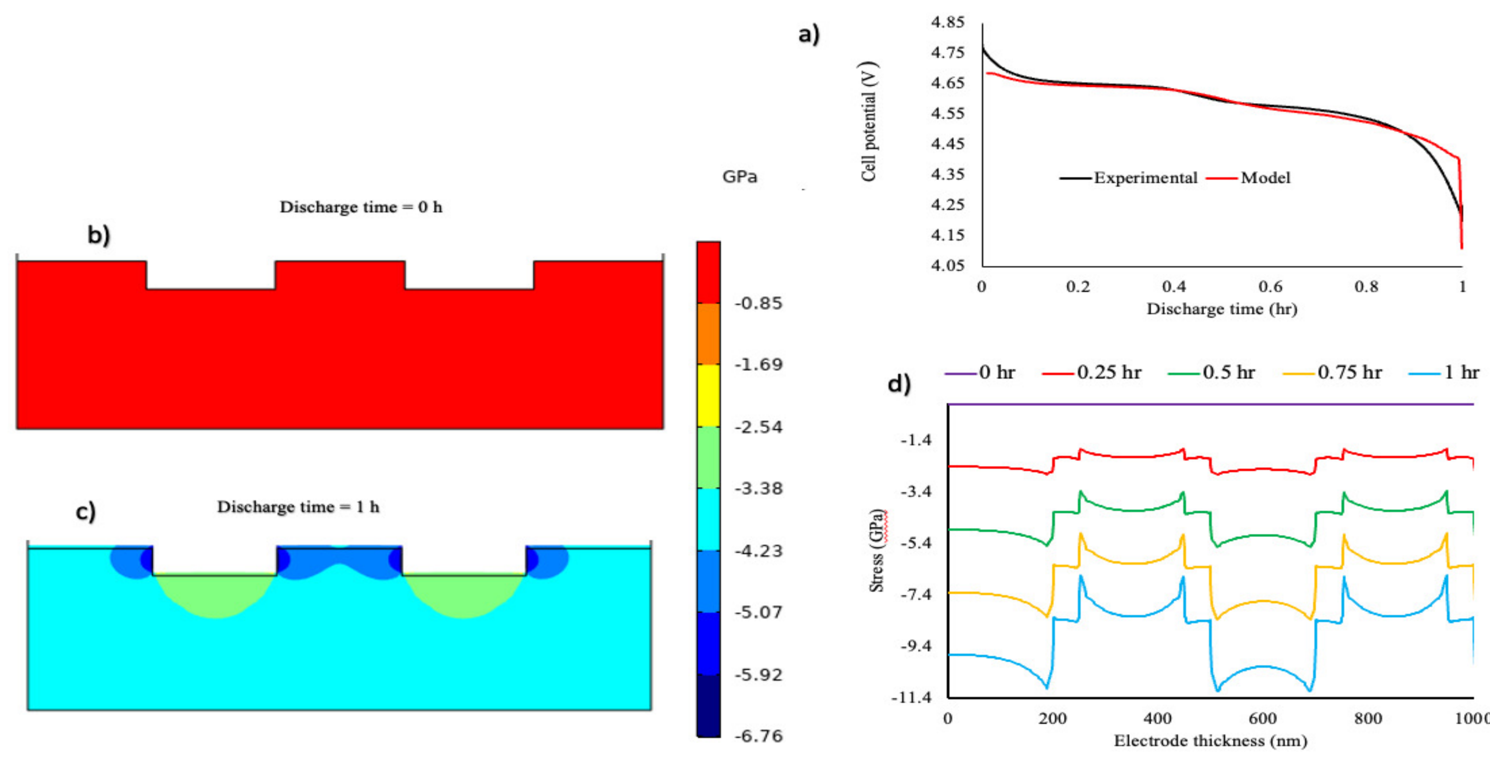

FIGURE 2. (a)discharge curve from experimental and modelling (b) Simulated mechanical stress profile at the discharge time of 0.1 h and c) 1 h (d) mechanical stress at interface for different discharge times of thin-film ASSLIB at 1C-discharge rate.

REFERENCES

1. Wu et al., Renewable and Sustainable Energy Reviews, 2019, 109, 367-385
2. Nie et al., Front. Chem., 2018, 6,
3. Zhu et al., J. Power Sources, 2022, 544, 231852
4. Zhu et al., JPCC, 2019, 123, 230046

VUB VRIJE UNIVERSITEIT BRUSSEL

VLAIO SIM Clusters for Growth

Excerpt from the Proceedings of the COMSOL Conference 2023 Munich