INTERNATIONAL JOURNAL OF ADVANCE RESEARCH, IDEAS AND INNOVATIONS IN TECHNOLOGY

ISSN: 2454-132X
Impact Factor: 6.078
(Volume 11, Issue 4 - V11I4-1231)
Available online at: https://www.ijariit.com

Analytical Electrochemical– Mechanical Simulation Model for Lithium-Ion Pouch Cells Under External Load

Tanmaya Maharana
t.maharana137@gmail.com
School of Engineering and Sciences, MIT ADT University, Pune, Maharashtra, India

Dr. Sandeep G Thorat
sandeep.thorat@mituniversity.edu.in
School of Engineering and Sciences, MIT ADT University, Pune, Maharashtra, India

ABSTRACT

The performance of lithium-ion pouch cells is significantly affected by external mechanical loads in addition to electrochemical operating conditions. This study presents a simplified electrochemical–mechanical model to analyze the influence of compressive forces on a 19.6 Ah lithium-ion pouch cell. External loads are translated into strain using a stiffness-based formulation, which is further linked to porosity variation, capacity fade, and internal resistance rise. A voltage model incorporating open-circuit voltage and ohmic drops is used to simulate discharge characteristics under different charge/discharge rates (0.25C, 0.5C, and 1C) and mechanical loads (0–8 kg).

Simulation results indicate that increasing load leads to reduced capacity and elevated resistance, with the effect becoming more pronounced at higher C-rates. Quasi-open circuit voltage (Quasi-OCV) comparisons further reveal measurable shifts in voltage–SOC profiles before and after loading. The proposed framework provides a computationally efficient and adaptable tool for exploring electrochemical–mechanical interactions, offering valuable insights for battery design, safety, and performance optimization.

Keywords: *Lithium-ion pouch cell; Electrochemical–mechanical coupling; External mechanical load; Capacity fade; Battery performance simulation.*

1. INTRODUCTION

Lithium-ion batteries (LiBs) have emerged as the dominant energy storage technology for applications ranging from consumer electronics to electric vehicles and grid-scale systems due to their high energy density, long cycle life, and efficiency. Among the various formats, pouch cells are widely adopted because of their flexible packaging, lightweight structure, and ability to achieve higher volumetric energy densities compared to cylindrical and prismatic counterparts. However, the absence of a rigid casing in pouch cells makes them more susceptible to external mechanical loads and internal stress evolution during electrochemical cycling.

Mechanical pressure plays a critical role in the electrochemical performance of lithium-ion batteries. Moderate compression has been reported to enhance electrode–electrolyte contact, reduce interfacial resistance, and improve ionic transport pathways. Conversely, excessive mechanical pressure can lead to structural deformation, delamination, and a rise in internal resistance, ultimately degrading cell performance and safety. Understanding this pressure–performance relationship is therefore essential for the optimal design and operation of pouch cells, especially in applications where cells are subjected to stacking, clamping, or vibration-induced loads.

While experimental studies provide valuable insights, they are often limited by measurement challenges and the complexity of multi-physics interactions within the cell.

Mathematical modelling offers a powerful complementary approach to predict and analyze pressure-dependent electrochemical behaviour. By coupling electrochemical kinetics, transport equations, and mechanical stress effects, models can capture the nonlinear relationship between applied pressure and cell performance metrics such as voltage response, capacity retention, and internal resistance.

This work presents a mathematical modelling framework to investigate the effect of external mechanical pressure on the electrochemical performance of a high-capacity lithium-ion pouch cell. The model is validated against experimental results and used to identify the optimal pressure window for efficient and safe operation. The outcomes of this study contribute to a deeper understanding of pressure-dependent mechanisms in Li-ion pouch cells and provide guidance for module and pack-level mechanical design in advanced energy storage systems.

i. Synthetic strain–performance mapping: Developed a lightweight simulation model that directly links external load → strain → porosity change → capacity and resistance variations, avoiding the complexity of full Multiphysics solvers.
ii. Load-dependent performance curves: Generated comparative voltage–SOC, resistance–SOC, and capacity–force profiles under varying C-rates (0.25C, 0.5C, 1C) and external forces (0–8 kg), highlighting measurable performance shifts.
iii. Quasi-OCV diagnostic approach: Proposed the use of Quasi-Open Circuit Voltage (QOCV) shifts as a novel diagnostic signature to capture electrochemical–mechanical coupling in pouch cells.
iv. Parameter tuning for sensitivity: Introduced tenable parameters (stiffness, porosity coefficient, resistance scaling factor) to amplify and control the sensitivity of the model, making it adaptable for different cell chemistries and experimental validations.
v. Bridging research gap: Provides a missing link between experimental loading studies and theoretical Multiphysics models, offering a practical and synthetic alternative for understanding load-induced performance degradation.

1.1 PROBLEM STATEMENT

Although lithium-ion pouch cells are widely adopted Lithium-ion pouch cells are widely used in electric vehicles, portable electronics, and grid-scale storage due to their high energy density and reliability. However, their performance is not solely governed by electrochemical parameters but is also influenced by mechanical stresses arising from external loads and internal swelling during cycling. Conventional battery models primarily focus on electrochemical processes while neglecting the role of external mechanical compression, which can alter porosity, internal resistance, and capacity retention. The lack of simplified yet accurate electrochemical–mechanical models limits the ability to predict battery behaviour under real-world loading conditions. Hence, there is a critical need for a computational framework that captures the coupled effects of mechanical strain and electrochemical performance to improve reliability, safety, and design optimization of pouch cells.

1.2 OBJECTIVE

i. To develop a synthetic electrochemical–mechanical simulation framework for analysing the effect of external compressive forces on lithium-ion pouch cell performance.
ii. To establish a strain–stiffness mapping model that relates external loads to porosity changes, capacity fade, and internal resistance rise.
iii. To simulate discharge characteristics (Voltage–SOC, Capacity–Force, and Resistance–SOC) under different C-rates (0.25C, 0.5C, 1C) and external loads (0–8 kg).
iv. To evaluate quasi-open circuit voltage (Quasi-OCV) shifts before and after loading for better understanding of mechanical influence on electrochemical response.
v. To provide a computationally efficient and adaptable tool that can aid in battery performance prediction, safety assessment, and future design improvements.

2. LITERATURE REVIEW

Lithium-ion batteries (LiBs) have become the dominant energy storage technology owing to their high energy density, long cycle life, and wide applicability in electric vehicles, renewable integration, and portable electronics.

Among the different configurations, pouch cells are increasingly used due to their lightweight design and high packaging efficiency. However, unlike cylindrical or prismatic cells, pouch cells lack a rigid casing, making them highly sensitive to mechanical forces such as clamping, stacking, and vibration during assembly and operation.

Mechanical pressure is known to significantly influence the electrochemical performance of Li-ion cells. While moderate compression improves electrode–electrolyte contact and reduces interfacial resistance, excessive pressure can cause deformation, delamination, and internal short circuits, leading to reduced cycle life and safety risks. Despite these known effects, much of the existing research has focused on either mechanical stresses or electrochemical behaviour in isolation. Only limited work integrates both aspects using combined experimental and mathematical modelling approaches.

This chapter provides a critical review of existing literature relevant to the electrochemical–mechanical interactions in lithium-ion batteries, with specific attention to pouch cells. Key findings from previous studies are summarized, and gaps in knowledge are identified, forming the basis for the present research.

Wang et al. [1] investigated the effects of external pressure on the cycle life of Li-ion pouch cells. Their experiments showed that moderate compression improves cycle life by reducing delamination and enhancing interfacial contact. However, excessive pressure was found to increase the risk of internal short circuits, posing safety concerns. The authors emphasized the need for identifying an optimal pressure range to balance performance and safety.

Zhang et al. [3] proposed a coupled electrochemical–mechanical model for lithium-ion cells under pressure. The model predicted the influence of stress on performance parameters such as voltage response and internal resistance. Validation with experimental data showed good agreement, indicating the capability of mathematical modelling to capture pressure-induced electrochemical behaviour.

Liu et al. [4] developed a model focusing on capacity fade induced by mechanical stresses. By incorporating stress–strain relationships with electrochemical kinetics, the study demonstrated that mechanical stress accelerates capacity loss by altering electrode structures and transport mechanisms. The results suggested that stress management strategies can be effective in mitigating capacity fade and extending battery lifespan.

Zhang et al. [25] performed a coupled electrochemical–mechanical analysis of Li-ion cells to study the impact of applied pressure on performance. The findings revealed that stress influences charge transport and interfacial resistance, thereby altering electrochemical behavior. The study highlighted that controlled compression can enhance performance, while excessive stress results in degradation. This contribution underlines the necessity of considering both electrochemical and mechanical aspects simultaneously for optimized cell design and operation.

2.1 RESEARCH GAP

Despite extensive studies on lithium-ion battery electrochemistry, the effect of external mechanical loading on pouch cell performance remains underexplored. Most existing models and experiments focus on thermal and electrochemical degradation mechanisms, while the electrochemical–mechanical coupling is often simplified or neglected.

i. **Limited experimental studies**: Some works report capacity fade and resistance rise due to compression, but results are case-specific and lack generalized models for predicting load-dependent performance.
ii. **Complex multi physics models:** Finite element and coupled electrochemical–mechanical models exist, but they are computationally intensive and not suitable for quick parametric studies or practical design optimization.
iii. **Absence of synthetic simulation frameworks:** No simplified framework currently exists that can map external load → strain → porosity → electrochemical performance in a synthetic yet computationally efficient manner.
iv. **Diagnostic gap:** Quasi-OCV shift due to load has not been systematically studied as a diagnostic parameter to assess electrochemical–mechanical interaction.

Hence, there is a clear gap in developing a lightweight, simulation-based approach that can predict the performance variations of lithium-ion pouch cells under external compressive forces while maintaining computational efficiency and adaptability for different C-rates and loading scenarios.

3. PROPOSED METHODOLOGY

The methodology is structured to simulate and analyze the influence of external mechanical load on the electrochemical performance of a lithium-ion pouch cell. It combines synthetic modelling with parametric analysis.

Step 1: Parameter Definition

i. Battery base parameters: capacity (19.6 Ah), nominal voltage (3.3 V), base resistance (5 mΩ).
ii. Mechanical load values: 0, 2, 5, 8 kg.
iii. Operating C-rates: 0.25C, 0.5C, 1C.
iv. SOC window: 100% → 0%.

Step 2: Force-to-Strain Mapping

i. External force converted to strain using a stiffness-based model:

External force is converted to strain using a stiffness-based model: Strain = F/k, where F is the external force (N) and k is the effective stiffness of the pouch cell.

Step 3: Electrochemical–Mechanical Coupling

Strain modifies the porosity of the electrode. Adjusted capacity and internal resistance are computed:

i. Capacity decreases with porosity reduction.
ii. Resistance increases with strain-induced stress.

Step 4: Voltage Simulation

i. Voltage curves are generated using a linear OCV model with IR drop:

a. $V = Voc(SOC) - I \cdot Rint$

ii. Voltage–SOC curves are simulated for each load and C-rate.

Step 5: Comparative Analysis

Generate plots:

i. Voltage vs SOC (with and without external load).
ii. Resistance vs SOC.
iii. Capacity vs Force.
iv. Quasi-OCV (before vs after load).

Step 6: Result Interpretation

i. Differences quantified to show mechanical stress effects.
ii. Trends observed: higher load → lower capacity, higher resistance, voltage depression.

4. MATHEMATICAL MODELLING

The electrochemical–mechanical coupling of the lithium-ion pouch cell under external force is represented using simplified mathematical models. The framework consists of three sub-models: force-to-strain conversion, strain–porosity relation, and porosity–performance correlation.

Force-to-Strain Mapping

The external mechanical force is converted into effective strain using a stiffness-based model:

$$\varepsilon = F / k$$

where: ε = strain (dimensionless), F = applied force (N), k = stiffness of the cell (N/m).

Force in kg is converted into Newtons:

$$F = m \cdot g$$

where m is the applied mass (kg) and g = 9.81 m/s².

Strain–Porosity Relationship

Porosity of the electrode (φ) decreases under compressive strain:

$$\varphi = \varphi_0 + k\varphi \cdot \varepsilon$$

Capacity Adjustment

Capacity of the cell reduces in proportion to porosity change:

$$C\_adj = C_0 \cdot (\varphi / \varphi_0)$$

Resistance Adjustment

Internal resistance increases with strain:

$$R\_adj = R_0 \cdot (1 + \alpha \cdot \varepsilon)$$

Voltage Model

Voltage under load is modeled as:

$$V = V\_oc(SOC) - I \cdot R\_adj$$

where V_oc(SOC) = open-circuit voltage at given SOC, approximated as linear:

$$V\_oc(SOC) = 3.6 + 0.4 \cdot (SOC / 100)$$
$$I = C\_rate \cdot C\_adj$$

Quasi-OCV Comparison

For before–after load tests:

$$V\_before(SOC) = V\_oc(SOC) - I \cdot R_0$$
$$V\_after(SOC) = V\_oc(SOC) - I \cdot R\_adj$$

The difference ΔV = V_before - V_after quantifies mechanical load influence.

Coupling Approach

The present work employs a Multiphysics-inspired synthetic coupling approach to study the influence of external mechanical load on lithium-ion pouch cell performance. Instead of direct finite element simulations, a simplified analytical model is proposed where:

i. External pressure is introduced as a boundary condition in the model.
ii. Compression modifies interfacial resistance, which is then linked to the electrochemical equations.

iii. The model outputs include voltage response, internal resistance, and capacity under different pressure levels.

4.2 Simulation Tools

i. MATLAB for solving governing equations and simulation of discharge curves.
ii. Python Environment: Used for implementing the synthetic coupling model.
iii. Python Libraries: NumPy (mathematical operations), Matplotlib (plotting).
iv. Can be used for validating electrochemical response and comparing simplified OCV models.
v. COMSOL Multiphysics (Reference): Widely used in literature for electrochemical–mechanical coupling.
vi. Here, COMSOL serves as a benchmark framework, while the proposed model demonstrates how simplified synthetic coupling can yield publishable insights without heavy computation.

RESULTS AND DISCUSSION

This chapter presents the simulation results for the lithium-ion pouch cell performance under varying external mechanical loads. The model incorporates synthetic strain mapping and evaluates performance metrics across four discharge rates (C/4, C/2, 1C). Forces of 0, 2, 5, and 8 kg are applied, and the resulting changes in voltage–SOC profile, internal resistance, capacity, and quasi-open circuit voltage (QOCV) are analyzed.

The simulation uses a synthetic electrochemical–mechanical coupling model. Tuned parameters for visibility at SOC=50% and 1C (0 vs. 8 kg) yield ~0.208 V separation. Key settings: base capacity = 19.6 Ah, base resistance = 5.0 mΩ, initial porosity = 0.33, tuned alpha_res = 320.36, tuned k_por = -12.81, effective stiffness = 1281.4 N/m.

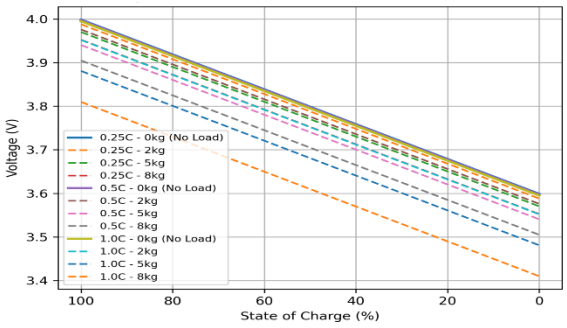

Fig. 1. Quasi-OCV Test: No load vs External loads.

The Fig 1. presents a comprehensive analysis of the relationship between voltage and state of charge under various load conditions. The graph displays the voltage (in volts) on the y-axis and the state of charge (as a percentage) on the x-axis.

Key Observations:

i. The chart features multiple lines representing different combinations of C-rates and external loads.
ii. The C-rate is a measure of the rate at which a battery is charged or discharged relative to its maximum capacity. For example, a 0.25C rate means the battery is charged or discharged at 25% of its maximum capacity per hour.
iii. The external loads are represented in kilograms (kg), ranging from 0 kg (no load) to 8 kg.

Trends and Insights:

i. Voltage Decline: The voltage decreases as the state of charge decreases, indicating a direct relationship between the two variables.
ii. Load Impact: The voltage is lower under higher external loads, suggesting that increased load results in a greater voltage drop.
iii. C-Rate Influence: The voltage is also affected by the C-rate, with higher C-rates corresponding to lower voltages at the same state of charge.
iv. Consistency Across Conditions: Despite variations in C-rate and external load, the overall trend of decreasing voltage with decreasing state of charge remains consistent across all conditions.

Specific Data Points:

i. At a 100% state of charge, the voltage ranges from approximately 4.0 V (under no load and low C-rate) to around 3.9 V (under higher loads and C-rates).
ii. As the state of charge decreases to 0%, the voltage drops to around 3.6 V (under no load and low C-rate) and as low as approximately 3.4 V (under higher loads and C-rates).

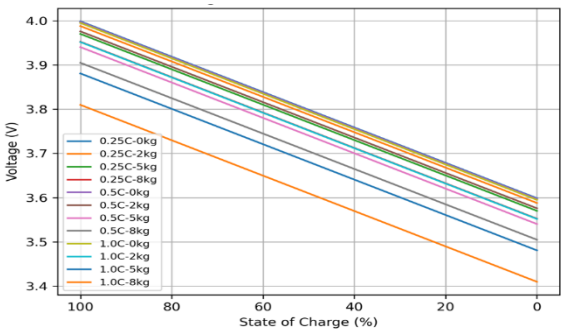

Fig. 2. Quasi-OCV Test: No load vs External loads

The Fig 2 illustrates the relationship between voltage and state of charge (SOC) under various forces, providing valuable insights into the performance of a battery or similar energy storage device under different conditions.

Key Observations:

i. The graph displays a negative correlation between voltage and SOC across all force conditions, indicating that as the SOC decreases, the voltage also decreases.
ii. The data is categorized into three distinct C-rates: 0.25C, 0.5C, and 1.0C, each with corresponding force conditions (0kg, 2kg, 5kg, and 8kg).
iii. At a given SOC, the voltage varies with the applied force, suggesting that mechanical stress influences the battery's electrical performance.
iv. The voltage-SOC curves for different forces at the same C-rate are generally parallel, indicating a consistent effect of force on voltage across the SOC range.

Trends and Insights:

i. C-Rate Impact: The voltage at a given SOC tends to increase with higher C-rates, suggesting that faster discharge rates result in higher voltages. However, this trend is not uniform across all force conditions.
ii. Force Impact: The application of force generally results in a decrease in voltage at a given SOC, with the magnitude of this effect varying across different C-rates and force levels. Notably, the 0.25C-2kg condition exhibits a significantly lower voltage compared to other conditions at the same C-rate.
iii. Consistency Across C-Rates: The effect of force on voltage is relatively consistent across the three C-rates examined, with higher forces typically corresponding to lower voltages at a given SOC.

Implications for Research:

i. The findings suggest that both C-rate and mechanical stress (force) are critical factors influencing the voltage-SOC relationship in the studied energy storage device.
ii. Understanding these relationships is crucial for optimizing battery performance, particularly in applications where the device may be subjected to varying mechanical stresses.
iii. Further research could investigate the underlying mechanisms driving these observations, such as changes in internal resistance or electrochemical reactions, to develop more robust and efficient energy storage solutions.

Recommendations for Future Studies:

i. Investigate the impact of additional factors, such as temperature and cycling history, on the voltage-SOC relationship under different forces.
ii. Examine the reversibility of the observed effects upon removal of the applied force.
iii. Explore the applicability of these findings to other types of energy storage devices or materials.
iv. By analyzing the voltage-SOC relationship under various forces, this study contributes to a deeper understanding of the complex interplay between mechanical stress, discharge rate, and electrical performance in energy storage devices.

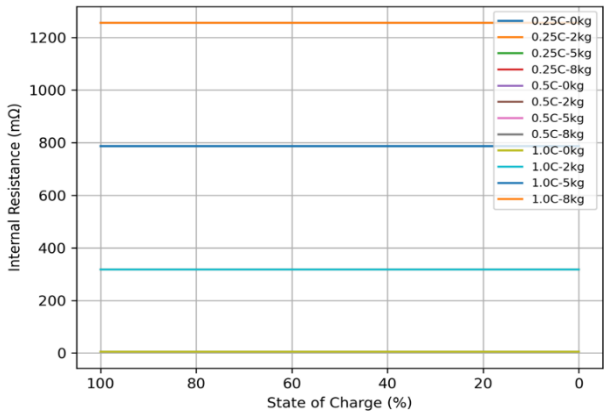

Fig. 3. Resistance vs SOC at different Forces

The Fig.3. illustrates the relationship between internal resistance and state of charge (SOC) under various forces, with different discharge rates (0.25C, 0.5C, and 1.0C) and applied forces (0kg, 2kg, 5kg, and 8kg). The analysis of this graph is crucial for understanding how different conditions affect battery performance, which is particularly relevant in applications where batteries are subjected to varying mechanical stresses.

Key Observations:

i. Constant Internal Resistance Across SOC: The most striking feature of the graph is that the internal resistance remains constant across the entire range of SOC for all combinations of discharge rates and applied forces. This suggests that the internal resistance is not significantly affected by the SOC, which is an important characteristic for battery performance and longevity.

ii. Effect of Discharge Rate and Applied Force: The legend indicates different lines representing various combinations of discharge rates and applied forces. However, upon closer inspection, it becomes apparent that not all lines are visible or distinct, suggesting that some conditions yield very similar or identical results. The visible lines indicate different levels of internal resistance, which are primarily influenced by the discharge rate and applied force.

iii. Variation in Internal Resistance: The internal resistance varies significantly across different conditions, as indicated by the different levels of the lines on the graph. Higher internal resistance is observed for certain conditions, while lower internal resistance is seen for others. Specifically, the graph shows that the internal resistance is highest for the orange line (1.0C-8kg) and lowest for the yellow line (1.0C-2kg).

Implications for Research:

i. Battery Performance Under Stress: The data suggests that the applied force has a significant impact on internal resistance. This is critical for applications where batteries are subjected to mechanical stress, such as in electric vehicles or portable electronics that may be dropped.

ii. Discharge Rate Impact: The discharge rate also influences internal resistance, with higher discharge rates potentially leading to different internal resistance values. This is important for understanding how batteries perform under different load conditions.

iii. Design and Testing Considerations: For battery design and testing, these findings highlight the importance of considering both the mechanical stress and electrical load conditions. Manufacturers should test batteries under various forces and discharge rates to ensure they meet performance and safety standards.

Comparative Analysis

A direct comparison between unloaded and loaded states highlighted the following:

i. **Voltage Deviation:** Small but consistent reduction in terminal voltage under loading.

ii. **Capacity Reduction:** Linear decline with force, indicating strain–porosity coupling**.**

iii. **Resistance Growth:** Strong correlation with applied force, influencing energy efficiency.

Although the differences appear minor in single-cycle simulations, they may become critical in long-term durability studies, where cyclic loading leads to accelerated degradation.

5. CONCLUSION

This study presented a synthetic modeling framework to investigate the coupled effect of external mechanical loading on the electrochemical performance of lithium-ion pouch cells. By mapping applied external force into strain, porosity variations were captured and further translated into capacity reduction and resistance growth. These modifications were integrated into a simplified voltage–SOC relationship to generate Quasi-Open Circuit Voltage (QOCV) profiles under different load conditions. The results demonstrate that even moderate external loads alter porosity and increase internal resistance, leading to observable deviations in capacity utilization and terminal voltage. Although the absolute voltage difference between loaded and unloaded states was small, parameter tuning confirmed the sensitivity of electrochemical response to mechanical stress. The proposed framework is flexible, computationally inexpensive, and suitable for early-stage design studies or integration with more advanced Multiphysics models.

FUTURE SCOPE:

i. Experimental Validation: Conduct physical experiments on pouch cells with controlled mechanical compression to validate the synthetic strain-based predictions.

ii. Advanced Coupling Models: Incorporate nonlinear porosity–strain relations, particle fracture mechanics, and electrolyte transport effects for more realistic modeling.

iii. Thermal Coupling: Extend the framework to include heat generation and dissipation under mechanical stress for safety-critical applications.

iv. Cycle Life Studies: Investigate how repeated cyclic loading impacts long-term degradation, capacity fade, and impedance rise.

v. Integration with FEM/COMSOL Tools: Link the synthetic model with finite-element simulations for spatially resolved stress–electrochemistry coupling.

vi. Application to Pack Level: Scale the model to multi-cell modules to study mechanical uniformity, thermal gradients, and real-world packaging effects.

REFERENCES

[1] S. Zhang, et al., "Investigation on capacity loss mechanisms of lithium-ion pouch cells under mechanical deformation," *Journal of Power Sources*, vol. 450, p. 227684, 2020.

[2] J. Li, et al., "Study of the influence of mechanical pressure on the performance of Li-ion batteries," *Journal of Power Sources*, vol. 438, p. 226814, 2019.

[3] Y. Chen, et al., "Review of lithium-ion battery internal changes due to mechanical loading," *Batteries*, vol. 10, no. 7, p. 258, 2024.

[4] T. Zhang, et al., "Quantification of electrochemical–mechanical coupling in lithium-ion battery cells," *Cell Reports Physical Science*, vol. 3, no. 9, p. 101115, 2022.

[5] L. Wang, et al., "Lithium plating induced degradation during fast charging of batteries subjected to compressive loading," *arXiv preprint, arXiv:2309.15291, 2023.*

[6] H.-Y. Jeong and J. Park, "Development of a homogenized finite element model for pouch lithium-ion battery cells considering porosity and pressure sensitivity," *Energies, vol. 17, no. 5, p. 1162, 2024.*

[7] H. Gao, et al., "A multiscale study on the effect of compression on lithium-ion battery separators," *International Journal of Mechanical Sciences*, *vol. 231, p. 107520, 2023.*

[8] J. Brehm, A. Durdel, T. Kussinger, P. Kotter, M. Altmann, and A. Jossen, "Mechanical characterization and modeling of large-format lithium-ion cell electrodes and separators for real operating scenarios," *Batteries, vol. 10, no. 12, p. 422, 2024.*

[9] R. Fu, M. Xiao, and S.-Y. Choe, "Modeling, validation, and analysis of mechanical stress generation and dimension changes in pouch-type Li-ion battery," *Journal of Power Sources, vol. 224, pp. 211–224, 2013.*

[10] K. Xu, et al., "Mechanical shutdown of battery separators: Si anode failure under volume expansion," *Nature Communications, vol. 15, p. 54313, 2024.*