Investigation of Mechanical Behavior of Lithium-ion Battery under Loading and Suggestion of Simplified Modelling Approach.

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1 Abstract

Ensuring battery safety is one of the key issues in the design of electric vehicles. In many cases, batteries are designed to be placed in strong cases or with sufficient clearance to prevent serious damage. On the other hand, to develop a vehicle which is lighter and can run longer, it is necessary to reduce the weight of battery cases and the clearance between cells. To meet the above requirements, it is important to fully understand the mechanisms leading up to the occurrence of short circuits that cause thermal runaway, and to feed such information back into the design.

Numerical analysis is one of the effective ways to evaluate battery cell deformation and damage. It requires an accurate understanding of the phenomena and the creation of an appropriate analytical model to reproduce it. However, a detailed and complex analytical model is computationally expensive, so it is desirable to build a simplified model to efficiently evaluate battery health in automobile collisions.

In this study, first, to clarify the mechanism of internal short circuit generation in a real battery cell, a test was devised that held it in a deformed state while the internal cross section was observed with a digital microscope. As a result, shear layers were observed in the cross section. Considering the appearance of shear layers to be the trigger for an internal short circuit, a detailed analytical model was constructed to reproduce this phenomenon, and the amount of strain, which is considered as the criterion for internal short circuit, was predicted from the analytical results. A simplified model of the battery cell was then constructed. Here, we focused on cell deformation, including buckling, that occurs under loads parallel to the direction of layer stacking, and created an analytical model to reproduce this deformation. The electrical characteristics were modeled using a randles circuit, and internal short circuits and heat generation were evaluated.

2 Introduction

Lithium-ion batteries (LIBs) have outstanding characteristics such as high energy density, long life, light weight, and high efficiency, and as a result they are widely used around the world as a sustainable energy source. Although LIBs for automotive applications have more stringent performance requirements than LIBs for consumer electronics, they are rapidly gaining popularity due to their recent performance improvements [1].

A lithium-ion battery (LIB) generally consists of a current collector, active material, and separator, and the separator acts as an insulator between the positive and negative electrodes to prevent short circuits. However, there is a risk of internal short circuits in automotive LIBs due to external shocks caused by collisions. When a short circuit occurs, the instantaneous flow of a large current generates heat, and in the worst case, there is a risk of thermal runaway [2]. To avoid such risks, measures such as placing energy-absorbing components around the battery module and providing appropriate clearances at key points are taken when designing electric vehicles (EVs) [3]. However, for the development of more competitive EVs, a leaner and safer design based on an understanding of the battery short circuit mechanism is required.

To solve the above issues, evaluation using numerical analysis is considered useful. As a numerical analysis method for batteries, LS-DYNA implements two methods: one using the LIB-EC model and the other using the Randles circuit model [4][5]. While the LIB-EC model is expected to be used for applications to predict battery performance from material composition, Randles circuit model is expected to be a simpler method to reproduce battery behavior. Earlier developments with the Randles approach included methods that model each layer of electrodes with solid or thick shell elements, however recently the keyword **`*EM_RANDLES_BATMAC`** was developed for analysis on a more macro scale [6]. **`*EM_RANDLES_BATMAC`** constructs fields representing positive and negative potentials at each node and connects them with a randles circuit. This allows for simple battery simulation without strictly constructing electrode layers. In addition, the internal resistance can be changed in response to outputs such as strain and stress, which can represent internal short circuits. In order to model internal short circuits in batteries through these functions, it is necessary to fully understand the mechanical mechanism of short circuit occurrence.

In this study, to clarify the mechanical mechanism of the internal short circuit, the battery was held in a deformed state, and the internal deformation was observed with a digital microscope. A detailed analytical model was then constructed to reproduce the phenomena observed in the experiment, and the hypothesis about the mechanism of internal short circuit was verified. The results of the analysis were used to estimate the internal short circuit criterion, which was then applied to a simplified battery crush analysis model using **`*EM_RANDLES_BATMAC`** to evaluate the internal short circuit and heat generation.

3 Experiments

3.1 Round Bar Compression Test

A round bar compression test of battery cell was conducted to investigate the mechanism of internal short circuit caused by external force. A prismatic automotive battery was disassembled and washed, and then re-stacked to make a laminated cell. The sample shape was 34.5 mm in diameter and about 6 mm in thickness. The specimen was statically compressed at 5 mm/min by a 10 mm diameter indenter. The outline of the specimen and the testing equipment, and the force-stroke curve are shown in Fig.1.

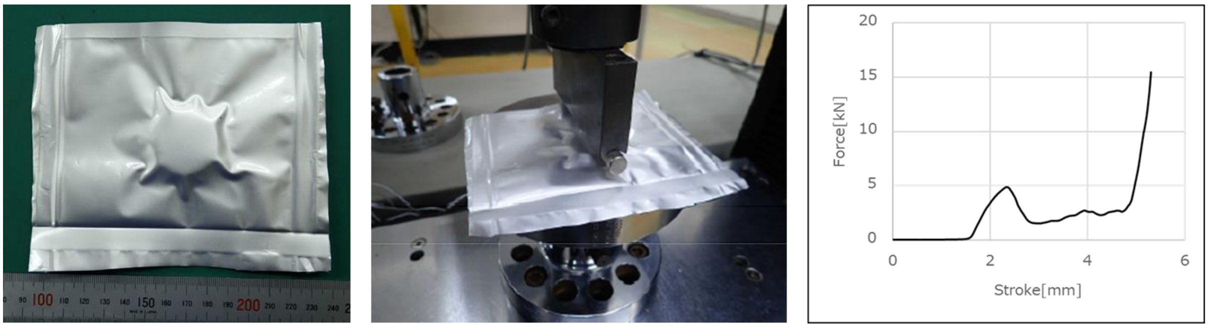

Fig.1: Specimen (Left), Testing Equipment (Center) and Force-Stroke Curve (Right)

3.2 Round Bar Compression and Relaxation Test

Referring to the force-stroke results of the round bar compression test, another specimen was statically compressed at 5 mm/min to a load of 4 kN (before the force drop-off) and then left under compression for approximately 18 hours until the stress relaxed. After stress relaxation, the specimen was cut and digital microscope photograph of the cross section shown in Fig.2 were acquired. A break in the layers can be seen in the center of the cell. Observing the enlarged view of the center of the cell shown in Fig.3 (Right), it can be seen that the center is not torn and separated, but each layer is shifted to the left or right. Small breaks can be seen in the alternating copper foil anode collector and the aluminum foil cathode collector. For the active material and separator, there was shear deformation and decrease in thickness, but no clear disconnection was observed. No disconnection or decrease in thickness of each layer was observed in the areas where the effect of loading was small, as shown in Fig.3 (Left). Assuming that the internally generated shear layers allowed the load to dissipate horizontally, the random misalignment between the layers could have reduced the load during compression.

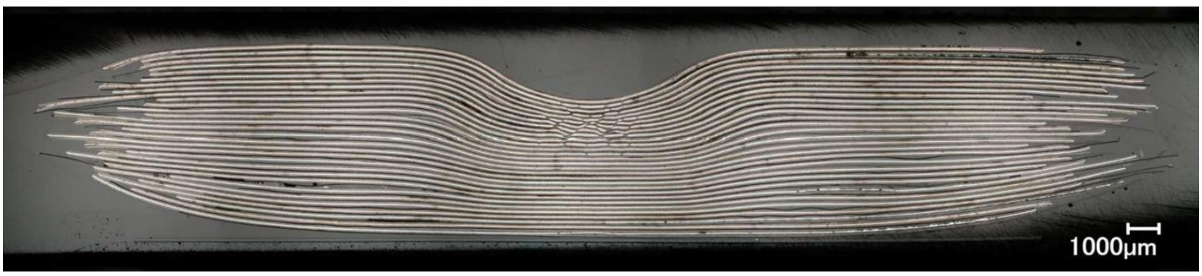

Fig.2: Cell Cross Section After Compression and Relaxation Test by Digital Micro Scope

Fig.3: Enlarged View of the Edge (Left) and Center (Right) of Cell Cross Section

3.3 Flat Plate Compression Test

A flat-plate compression test was performed to obtain the compression characteristics of the entire battery cell. Specimens were prepared as in the round bar compression test. However, the diameter was 17 mm and the height was about 10.4 mm. The specimen was statically compressed at 5 mm/min by a flat indenter. The outline of the specimen and the testing equipment, and the force-stroke curve are shown in Fig.4.

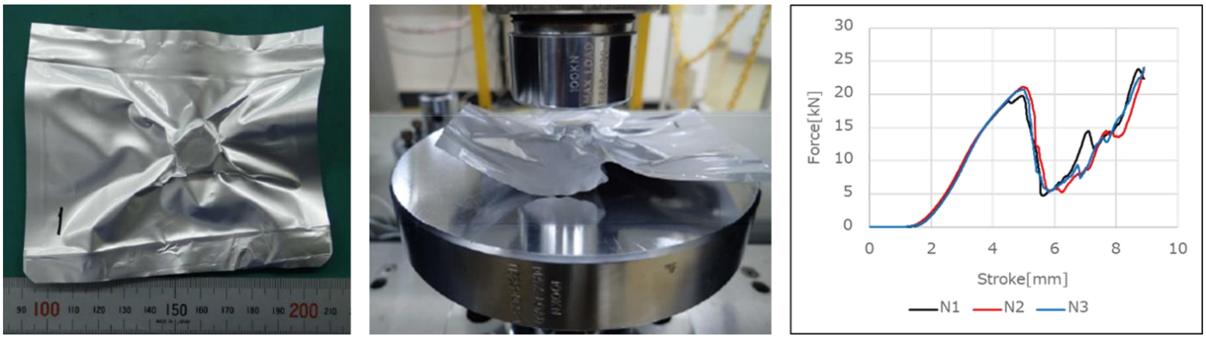

Fig.4: Specimen (Left), Testing Equipment (Center) and Force-Stroke Curve (Right)

3.4 Tensile Test

Tensile tests (test speed = 5.0 mm/min, grip interval = 50 mm) were performed on the anode and cathode collector and separator to obtain tensile characteristics. Test piece (JIS K6251 No. 3 dumbbell shape) was prepared by disassembling a prismatic automotive battery (See Fig.5). An image of the surface of the test piece during the test was acquired by a digital image correlation method system, and the stress-strain curve was determined (See Fig.6).

Fig.5: Dumbbell Test Piece Anode Collector (Left), Cathode Collector (Center) and Separator(Right)

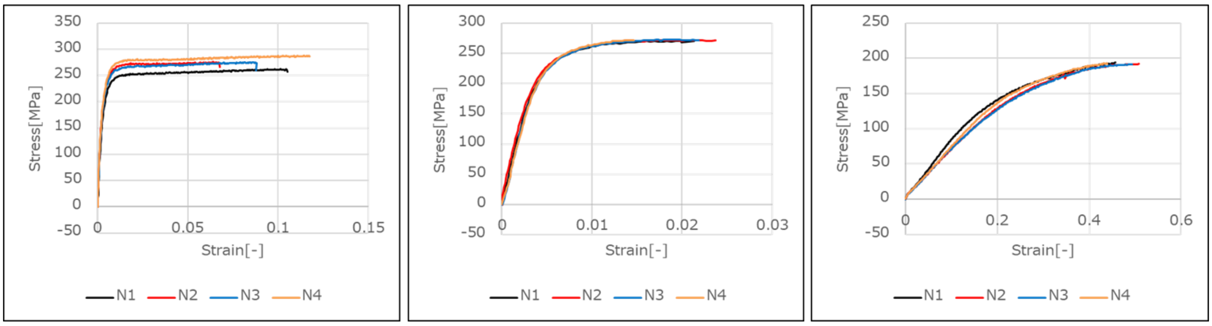

Fig.6: Stress-Strain Curve Anode Collector (Left), Cathode Collector (Center) and Separator(Right)

4 Numerical Simulation of Round Bar Compression Test

4.1 Model Description

We attempted to reproduce the appearance of shear layers observed in round bar compression test by analysis. Assuming a plane strain condition, the bar axial direction was modeled with a single element for simplicity (like a thick slice). The active material and separator, which are considered to have large out-of-plane deformation, are modeled by solid elements, while the current collector, which is considered to have more significant bending deformation than out-of-plane deformation, is modeled by shell elements. In order to reduce calculation time, both ends of the cell, which are considered to have little effect on the deformation of the center of the cell, were omitted, and the loading speed of the indenter was set to 10,000 times that of the actual phenomenon. Fig.7 shows an overall view of the analytical model and an enlarged view of each electrode layer, along with a cross-sectional view of the actual battery cell.

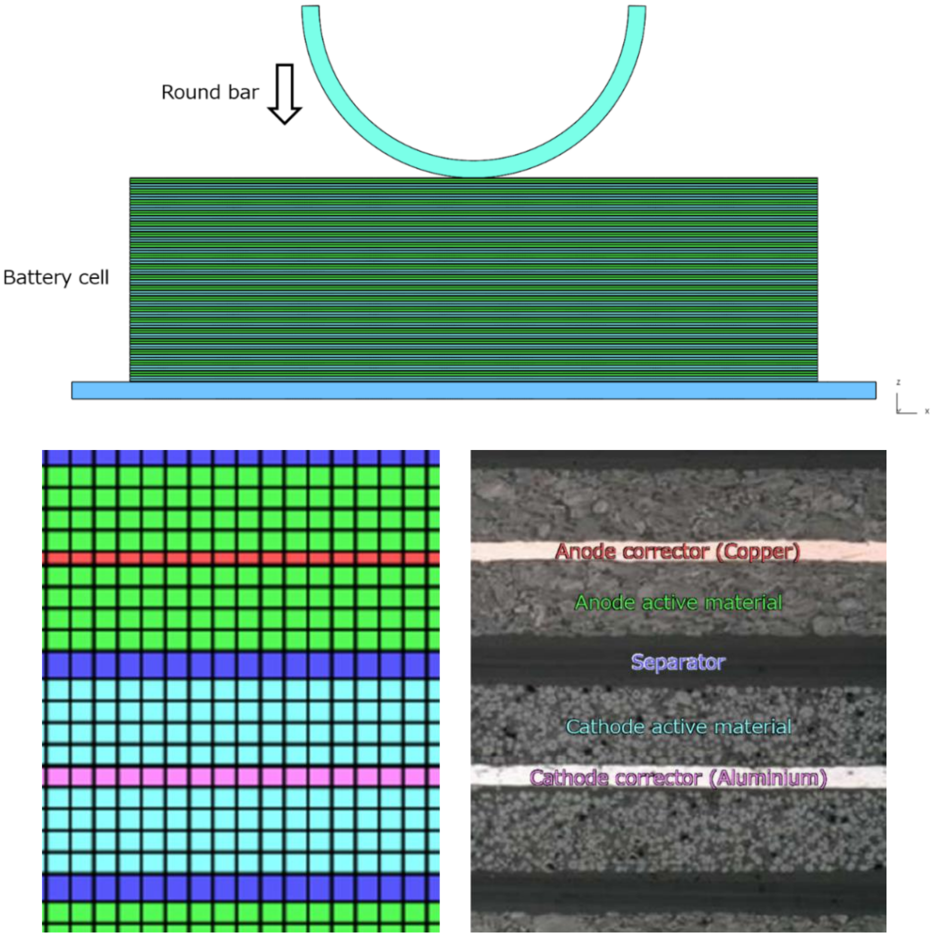

Fig.7: Overall View of the Analytical Model (Upper) and Enlarged View of Each Electrode Layer (Lower)

4.2 Material Properties

4.2.1 Current Collector

The current collector was modeled by ***MAT_PIECEWISE_LINEAR_PLASTICITY** assuming isotropy. Stress-strain characteristics were identified from tensile test results.

4.2.2 Separator

Separators were modeled by ***MAT_MODIFIED_HONEYCOMB** because they were considered to have different properties in tension and compression. Stress-strain property in the tensile direction was identified from tensile test, and that in the compressive direction were identified based on the results of flat-plate compression test. Since it is analytically expensive to reproduce the entire flat-plate compression test, an analytical model was created by cutting out one anode-separator-cathode electrode layer with a cross-sectional area of 0.1×0.1 [mm²], and the force-stroke was converted to stress-strain for evaluation. Since the separator was considered to be softer than the active material and deformed earlier in compression, we focused on the A-B section shown in Fig.8 and tuned the characteristics of the separator.

4.2.3 Active Material

Active materials were modeled by ***MAT_SOIL_CONCRETE** because they were considered to behave similarly to soil. ***MAT_SOIL_CONCRETE** allows the definition of a [pressure - von Mises stress] relationship that is similar to the Drucker-Prager model. The yield criterion for the Drucker Prager model can be approximated using the friction angle ϕ and the cohesion c in the Mohr Coulomb model as follows

$$\sqrt{J_2} + \eta p = \xi c$$

$$\eta = \frac{6\, sin\, \phi}{\sqrt{3}(3 - sin\, \phi)},\quad \xi = \frac{6\, cos\, \phi}{\sqrt{3}(3 - sin\, \phi)}$$

where J_2 is second invariant of the stress deviator, and p is pressure [7]. The friction angle ϕ was set to 20 [°] and the cohesion c to 30 [kN/m²], referring to the Mohr-Coulomb criterion values for common soil materials [8]. The [pressure-volumetric strain] relationship was tuned focusing on the B-C section of the flat plate compression test shown in Fig.8.

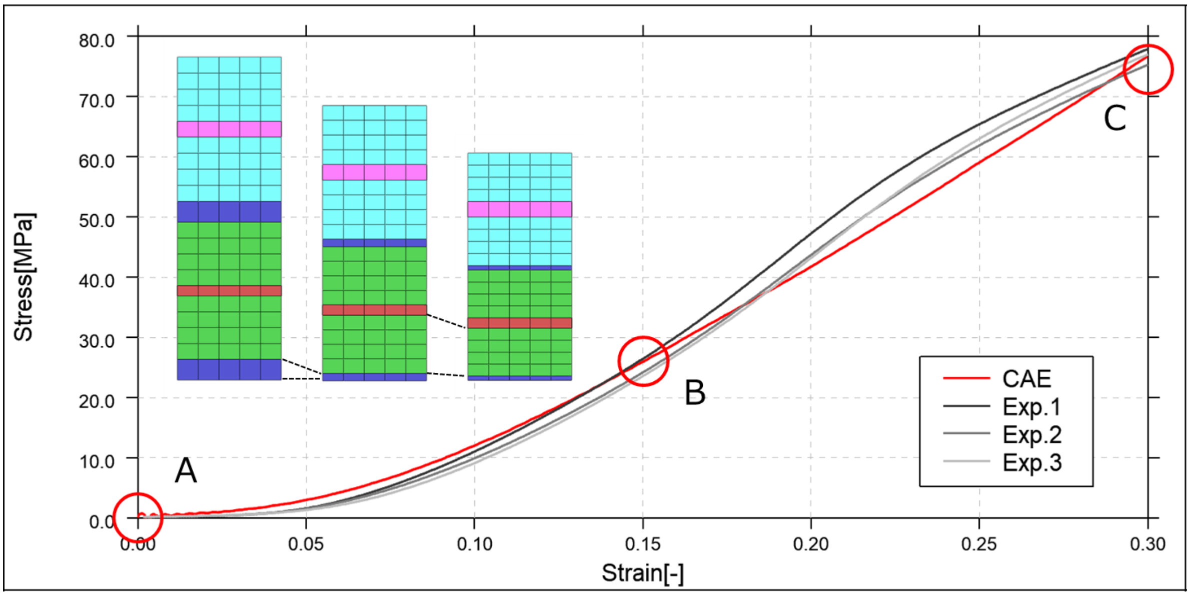

Fig.8: Compression Analysis Result of One Anode-Separator-Cathode Electrode Layer

4.3 Simulation Result

Fig. 9. shows the simulation result of cell deformation, and force-stroke curve compared with the experimental result. Since the analytical model was created with one element (0.025 mm) in the bar axial direction, the load values of the experimental data were scaled for comparison. The analytical result shows shear layers and loading history similar to the experiment. Observation of the trigger of the shear layers showed that the positive electrode collector was first ruptured, followed by the rupture of the negative electrode collector with large deformation of active material (See Fig.10). The onset of the shear layers stopped the load increase and eventually caused a sudden drop in load due to active material elements failure. The maximum value of the load was higher in the analysis, but this may be due to the boundary condition of plane strain, which restricts the degrees of freedom in the depth direction more strictly than in the real phenomenon. Based on the change in layer thickness that occurred from the initial condition to the onset of the shear layers, a macroscopic strain criterion of 0.28 was assumed to cause an internal short circuit and applied to the simplified analytical model shown in the following Chapter 5.

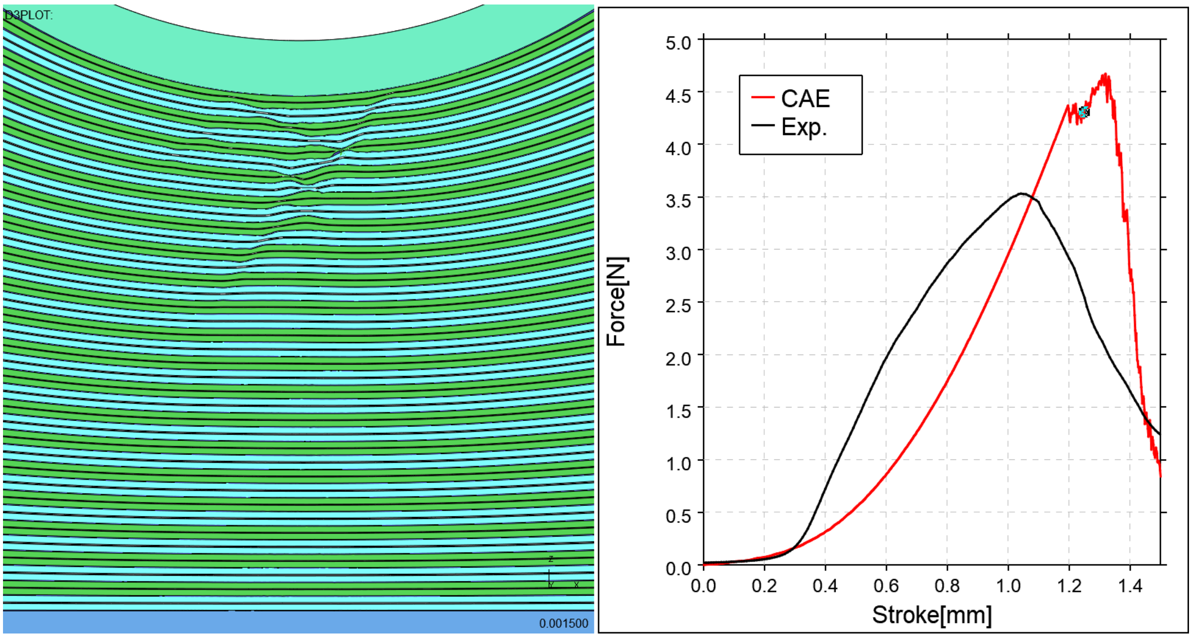

Fig.9: Simulated Cell Deformation (Left), Comparing Between Experiment and Simulation Force-Stroke Curve (Right)

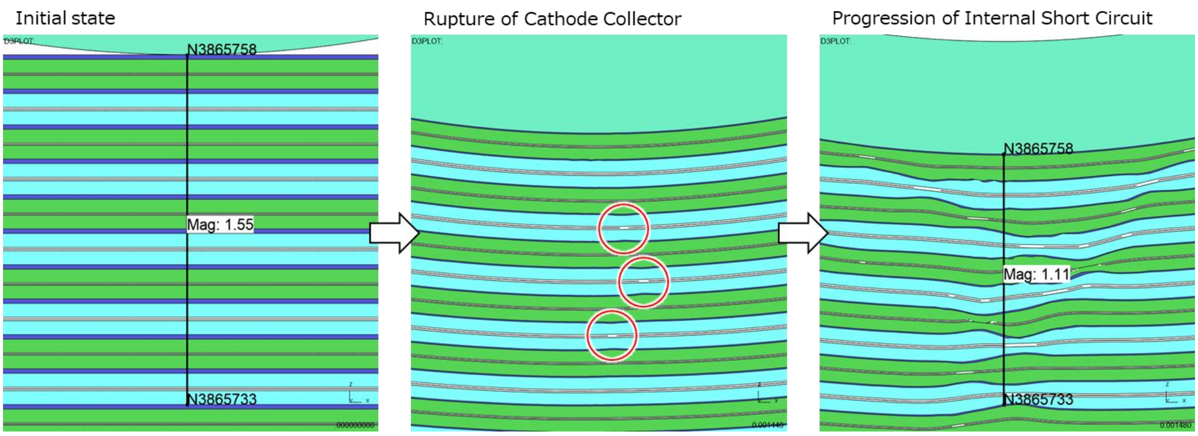

Fig.10: Mechanism of Internal Short Circuit Occurrence

5 Simplified Modelling Approach

5.1 Concept

The analysis conducted in Chapter 4 was aimed at exploring the mechanism of short circuit occurrence, and thus detailed modeling was performed for each layer of the cell. However, it is impractical from a computational cost perspective to apply such a detailed battery model to, for example, a vehicle crash analysis. For simplified battery modeling, a method using **`*MAT_CRUSHABLE_FOAM`** for mechanical properties and **`*EM_RANDLES_BATMAC`** and **`*EM_RANDLES_SHORT`** for electrical properties including internal short circuits has been proposed previously [9]. While such a simplified model is expected to be computationally very fast, it may have problems reproducing the deformation modes of the cell. In particular, battery cells are known to cause deformation, including buckling, when loaded parallel to the direction of layer stacking, and it is desirable that such deformation modes be reproduced in the simplified model as well [10]. In response to this issue, we studied the creation of an analytical model which can represent buckling deformation and the resulting internal short circuit in a relatively coarse element size.

5.2 Model Description

As shown in Fig.11, a prismatic battery cell was made with 2~3 mm elements, which is compressed in the in-plane direction by a rigid tool. The mechanical properties of the cell were modeled by a combination of **`*MAT_MODIFIED_HONEYCOMB`** (solid elements), **`*MAT_ELASTIC`** (shell elements) and **`*MAT_FABRIC`** (membrane elements). Shell and membrane elements are node-shared with solid elements, and shell elements are slightly offset in the out-of-plane direction. While the membrane elements add in-plane stiffness to the cell, the offset shell elements add out-of-plane bending stiffness to the cell without significantly affecting the in-plane stiffness (See Fig.12). By tuning these stiffnesses and offset amounts, the deformation mode of buckling and the resulting load balance in each direction can be adjusted. No validation studies were conducted in this study, and the various properties of the analytical model were made up as sample values. However, the internal short circuit criterion was defined as the amount of strain assumed in Chapter 4.

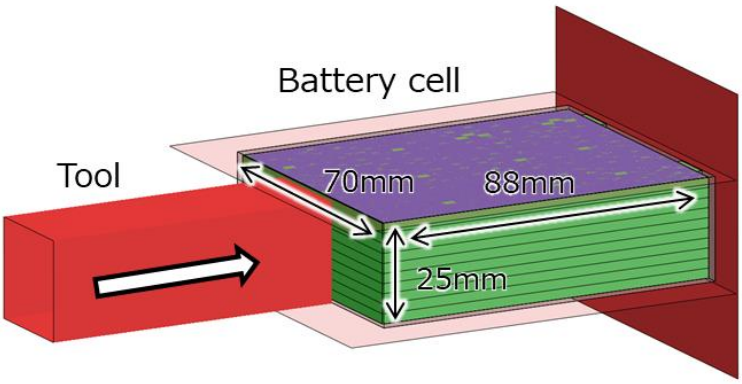

Fig.11: Overview of Simulation Model

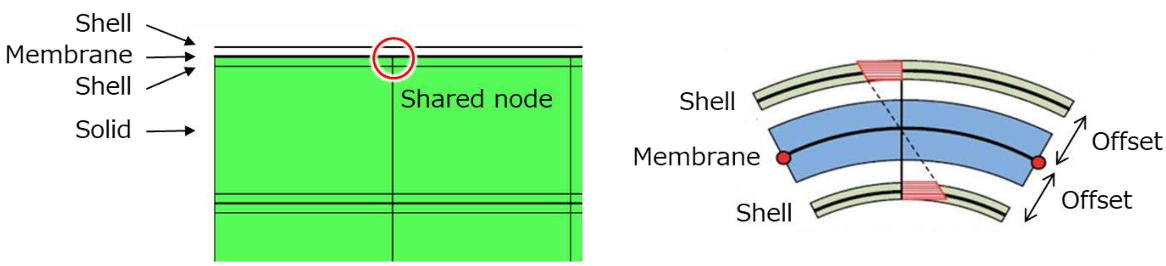

Fig.12: Shell, Membrane and Solid Combined Model

5.3 Simulation Result

Fig.13 shows the simulation results. The buckling deformation in the cell, the internal short circuit caused by the defined strain criterion, and heat generation were observed. Calculation time was about 110 minutes on 32 CPU. Future validation of this approach through comparison with actual experiments is desirable.

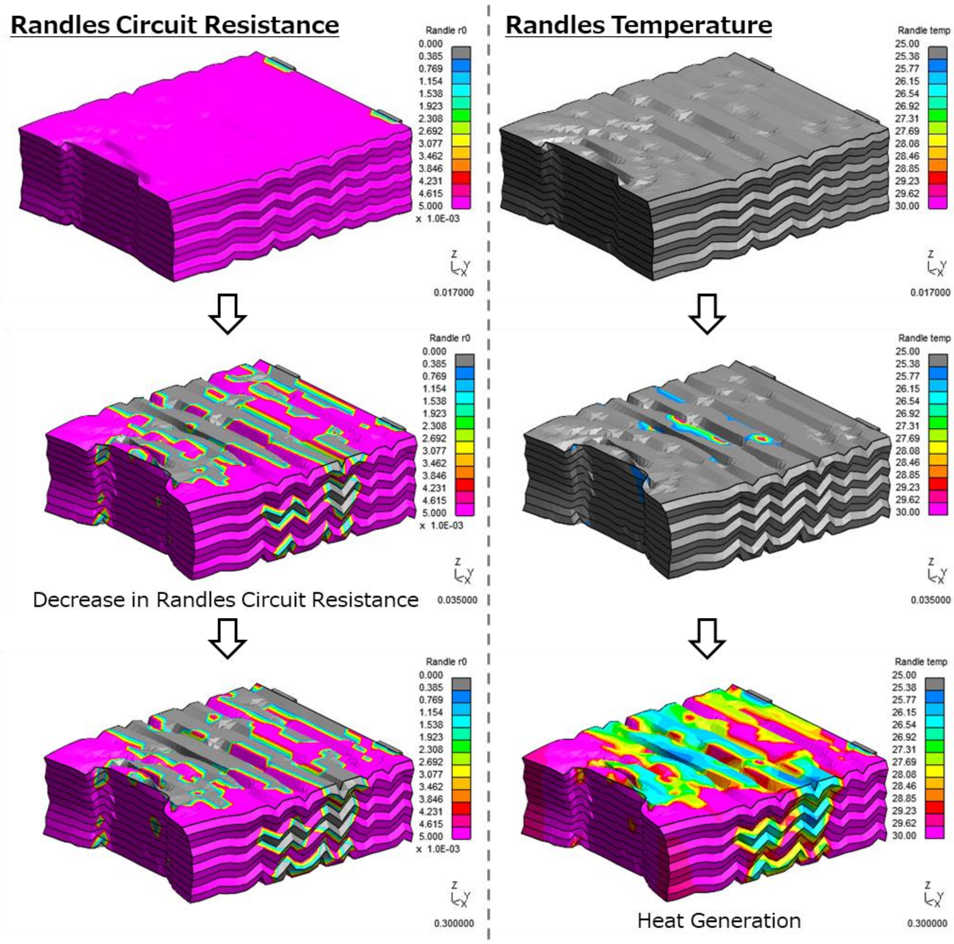

Fig.13: Decrease in Randles Circuit Resistance (Left), and Heat Generation (Right) due to Internal Short Circuit

6 Summary

In this study, we focused on the short circuit phenomenon of LIBs and investigated their mechanical behavior under loading. At first, some experiments were conducted to obtain the load histories and the cross section images of battery cells compressed by round bar. Then, a detailed analytical model was developed to reproduce the phenomena observed in the experiment, namely, the appearance of the shear layers and the decrease in load. From the results of the analysis, it was inferred that the trigger for the appearance of the shear layer, which is considered to cause an internal short circuit, is the rupture of the cathode collector (Aluminum). Based on the results, the macroscopic strain criterion for short circuit occurrence was also predicted. The predicted short circuit criterion was then applied to the suggested simplified battery analysis model. This simplified model is intended to represent buckling deformation caused by loads parallel to the cell stacking direction on low computational cost. From the simulation results, it was observed that the expected deformation modes were generated, which resulted in internal short circuits and heat generation.

For future prospects, the following studies are desired.

- Obtain accurate properties of the active material layer
- Improve accuracy and robustness of the analytical model that reproduce shear layer occurrence
- Conduct testing and validation for the simplified modelling approach

7 Acknowledgement

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8 Literature

[1] Masias, A.; Marcicki, J.; Paxton, W.A. "Opportunities and challenges of lithium ion batteries in automotive applications.", ACS energy letters 6.2, 2021, 621-630.
[2] Feng, X.; et al. "Thermal runaway mechanism of lithium ion battery for electric vehicles: A review.", Energy storage materials 10, 2018, 246-267.
[3] Belingardi, G.; A. Scattina. "Battery Pack and Underbody: Integration in the Structure Design for Battery Electric Vehicles—Challenges and Solutions.", Vehicles 5.2, 2023, 498-514.
[4] Im, K; et al. "Electrochemical-Thermal-Mechanical Coupling of Lithium-Ion Battery Model in LS-DYNA.", 16th International LS-DYNA Users Conference, 2020.
[5] L' Eplattenier, P.; et al. "A distributed Randle circuit model for battery abuse simulations using LS-DYNA.", 14th International LS-DYNA Users Conference, 2016.
[6] L' Eplattenier, P.; Çaldichoury, I. "BatMac: a battery macro model to simulate a full battery in an electric or hybrid car crash using LS-DYNA.", 12th European LS-DYNA Conference, 2019.
[7] Neto, EdS.; Perić, D.; Owen, DRJ. "Computational methods for plasticity: theory and applications.", John Wiley & Sons, 2011.
[8] Lukić, D. " Friction angle of soil and rock.", 6th International Conference Contemporary Achievements in Civil Engineering, 2018.
[9] Schwab, M.; et al. "Abuse characterization and simulation of battery cells and cell arrangements" 16th LS-DYNA Forum, 2022
[10] Ali, M. Y.; Lai, W. J.; Pan, J. "Computational models for simulations of lithium-ion battery cells under constrained compression tests." Journal of Power Sources 242, 2013, 325-340.