Compression Experiment and Simulation on Prismatic Lithium-ion Batteries

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Abstract. In order to understand the mechanical characteristics and failure modes of prismatic lithium-ion battery under mechanical loading conditions, flat plate compression and hemispherical punch indentation test were performed on 186570 prismatic LiFePO$_4$ lithium-ion batteries and bare cells (cells without shell casing). Load and displacement of the cells and bare cells were measured in all tests. Additionally, temperature and voltage of the battery cells were also recorded. In flat plate compression condition, the battery shell casing cracked and electrolyte was squeezed from the cells. In hemispherical punch indentation condition, the punch displacements were stopped when a drop in force and voltage of the cell, as well as a rise in temperature indicated an internal short circuit in the cell. From the measured load-displacement data of the bare cell under flat compression condition, the individual compression stress-strain curves were calculated for the bare cells and used to develop a finite element model for the prismatic LiFePO$_4$ battery. The bare cell is modeled as compressible foam material in LS-Dyna. This model can successfully predicted the load displacement relation of the cell under compression condition. On the other hand, this model can closely predict the force and punch displacement corresponding to the onset of short circuit in the cell under hemispherical punch indentation condition. The present tests and simulation can help to understand the deformation shape and internal short circuit mechanism of the prismatic lithium-ion cells under mechanical abuse conditions.

Introduction

Lithium-ion batteries as an energy storage have become widely used in passenger cars, public transportation and commercial vehicles [1]. On the other hand, they are still in the race for more energy density. Battery in a running vehicle is under various road conditions with speeds and accelerations, so it is exposed to local sophisticated loading and deformations, and in extreme cases, such as crash, can result in local damage of the cell and lead to short circuit, fire or explosion. So safety of the battery is key to the electric vehicle safety. According to the present research on lithium-ion battery safety, more focuses are on electrochemistry, thermal management than mechanical integrity. The electrochemistry and thermal properties for lithium-ion cell have been widely studied so far by nail penetration or pinch tests [2-4]. But the influence factor and mechanism of mechanical safety is still not clear enough. Besides, the mechanical abuse tests and evaluation in battery safety standards still stay in the stage of qualitative judgment and doesn’t consider the force, voltage and temperature in testing process [5]. So it’s not enough to definitely understand the mechanical behavior of the battery under mechanical loading conditions. The need to better understand the mechanical behavior of prismatic lithium-ion batteries under mechanical abuse conditions that may lead to electric short circuit and mechanical failure has motivated this research.

According to literatures, Sahraei and Wierzbicki [6-8], Fehrench [9] Xu Jun [3, 10], Zhang Tao [11], and Zhang Dazhi [12] et al. have done much studies on mechanical properties and internal short circuit of 18650 cylindrical cells and pouch cells. Sahraei and Wierzbicki [7] studied the mechanical properties of a small pouch cell in several loading conditions by using an extensive
experimental program and developed a numerical model to predict the properties observed during the tests. In their later study [8], they used homogenous isotropic crushable foam material to develop finite element (FE) models for 18650 cylindrical cells, and that predicted the load-displacement properties and the deformation levels to cause internal short circuit. Sahraei didn’t consider the state-of-charge (SOC) as an influence factor of cell’s mechanical properties under quasi-static loading conditions. However, Xu Jun developed an anisotropic homogeneous model of the 18650 cylindrical cell describing the jellyroll while using compression, indentation, and bending tests at quasi-static loadings. In Xu jun’s model, SOC dependency of the lithium-ion battery is further included through an analogy with the strain-rate effect. Moreover, with consideration of the inertia and strain-rate effects, the anisotropic homogeneous model is extended into the dynamic regime and proven capable of predicting the dynamic response of the lithium-ion battery using a drop-weight test. The established model can improved accuracy compared to homogeneous isotropic models.

The above writers mainly concentrated on features and constitutive model of cylindrical cells and pouch cells, but they ignored the influence of shell casing on cells [4, 6-8]. Because mechanical abuse test on battery is dangerous and complexity of internal structure make it difficult to find a common constitutive model for the mechanical property of all lithium-ion battery, so this paper mainly focus on mechanical properties and mechanical conditions that lead to a short circuit or shell casing cracking of Li-ion battery, especially on prismatic Li-ion battery. With the expanding of the electric vehicle (EV) market in China, prismatic LiFePO$_4$ cell is more and more widely used in BYD E6, ZD D2 and so on, because of its higher energy density in battery pack, easier for assembly and management than cylindrical and pouch cells in vehicles. So the safety of prismatic cell is need to understand, but the literatures about mechanical properties of prismatic cell are limited. The shell casing and interior structure of the prismatic battery is much different to the cylindrical and pouch cell, which lead to the difference in mechanical properties of them, so the main object of this paper is to demonstrate the mechanical properties, deformation shapes and internal short circuit mechanism of 186570 prismatic LiFePO$_4$ lithium-ion battery under flat plate compression and local indentation loading. Finally, a homogeneous isotropic compressible foam material was chosen to model the bare cell of prismatic cells in LS-Dyna and it can successfully predict the load-displacement relation and deformations leading to short circuit of the cells. The present tests and simulation can help to understand the deformation shape and internal short circuit mechanism of the prismatic lithium-ion cells under mechanical loading conditions.

**Structure of the Cells**

The cells used for this research is 186570 prismatic LiFePO$_4$ lithium-ion cell with 5 Ah capacity, 3.2 V voltage, and have dimensions of 18 mm×65 mm×70 mm, which is different from cylindrical and pouch cell in shell casing and interior structure, as shown in Figure 1, Figure 2 and Figure 3.

Vernier caliper was used to measure the size of the cell and thickness of the shell casing. The thickness of the side shell casing is 0.5 mm and the bottom is 1.1mm thicker. The side and bottom shell casing is an integrated structure, welded by a 1.6mm thick top-cap. The interior of the cell is a multilayered structure, consisting of anode (negative electrode), cathode (positive electrode), polyolefin separator and current collectors made by aluminum foils and copper foils. The feature of 186570 prismatic LiFePO$_4$ Li-ion cells is that the electrodes/separators assembly is stacked of cards instead of wound in cylindrical cells and fold in the pouch cells. Firstly, the active particle with binder was firmly adhered to the metallic foils, which is called positive electrode and negative electrode. The separators are made as a pocket, than the positive electrodes are inserted into the separators pocket and stacked together with negative electrodes. Finally, the cells are injected with electrolyte which is a bridge for Li-ion between anode and cathode. There are 48 layers of the positive electrodes, 50 layers of the negative electrodes and 98 layers separators stacked together in a 186570 prismatic Li-ion cell. From the view of manufacturing process, the fold structure and jelly
roll structure means that there is only a single cell in pouch and cylindrical battery. But the stacked structure means that there are 48 micro-cells connected in parallel in a prismatic battery. So the internal short circuit of prismatic cell is much different from pouch and cylindrical cell when facing the mechanical loading, and this is what this paper of interest.

Test on Prismatic Cells
The instruments used for this research include Microcomputer Control Mechanical Testing Machine (MCMT), and Agilent Data Collector System (ADCS). MCMT is used to measure the loading force and displacement in the process of flat plate compression and hemispherical indentation. ADCS is used to record the voltage and temperature. Flat compression between two plates and indentation with a hemispherical punch were performed on battery cells and bare cells. All the cells were discharged to less than 5% State of Charge (SOC) to prevent extreme reactions during the tests. In all cases, the crosshead speed was 1 mm/min and loading direction is through the thickness direction (Z direction), shown as Figure 4.

Flat Compression on Bare Cells
The objective of flat compression on bare cells (by removing shell casing) is to extract the stress-strain curve of it. In this condition, the bare cell was compressed between two plates until the force reached 350 kN, as shown in Figure 5.
In this case, only load-displacement was measured, as shown in Figure 6 (left). In the loading process, the electrolyte was squeezed from the bare cell. The porosity of the active particles could be as high as 60% with the voids typically filled with electrolyte [7]. So no visible increase in the lateral dimension of the specimen was observed. This suggests a very low Poisson ratio of the cell material, so a model of compressible foam could be used in the numerical simulation model [6-8]. Because there is very little deformation in lateral dimension, the relationship between the average stress (\( \sigma \)) and volumetric strain (\( \varepsilon \)) can be calculated by formula (1), where \( P \) is the loading force and \( A \) is the contact area between plate and bare cell. Also, note that \( H \) is the flat platen downward displacement and \( H_0 \) is the initial size of the bare cell in the Z direction (the thickness of bare cell).

\[
\sigma = \frac{P}{A}, \quad \varepsilon = \frac{H}{H_0}
\]

According to the formula (1), the measured load-displacement curves were converted into stress-strain of the individual components, as shown in Figure 6 (right). As seen in engineering stress-strain curve, the maximum slope of the curve is 350MPa. This value is very important and the curve will be used to establish the finite element model in section 4.

Flat compression on battery cells.

The test of compression between two plates on battery cell and result is showed in Figure 8. Voltage and temperature were also measured as well as load-displacement in this case. The thermocouple was pasted in the side of the cell case. The measured load-displacement relation, voltage-time and temperature-time is shown in Figure 9 and Figure 10.
The Figure 8 shows that the curve of load-displacement has three obvious stages. In the first stage, the force increasing suddenly is due to shell casing resistance. The second stage is a platform stage because of densification of porosity active material in the cell. At the end of second stage, top-cap was broken and the electrolyte was squeezed from the cell. As shown in Figure 9, the broken displacement is 2.95 mm. Almost at the same time, the voltage dropped from 3V to zero and temperature rise from 22.2 °C to 24.8 °C, shown in Figure 10. The changing point of the voltage and temperature is at 188s, which is equal to the 3.13mm displacement delaying little than the displacement of shell casing crack. After many times repeated experiment, we can draw a conclusion that the crack of the shell casing causes the drop of the voltage. When the shell casing cracked, the “bridge” connecting anode and cathode would break, so the electric circuit is broken. However, there are some active material left in the electrolyte, so the active material would react together and release a small amount of heat that leads to the temperature rising.

The third stage of the load-displacement curve is a plastic hardening process. In this stage, the cell continue to be harder and harder. Force increased as linear growth until the force reached 350
kN. It is worth mentioning that the force didn’t drop before the end of the test, which demonstrated the interior material didn’t yield under plate compression condition. Conclusion shows that the cell under a large area compression loading condition would cause the shell casing crack and the leakage of the electrolyte, but no internal short circuit occur and the temperature rise is little because the SOC is lower than 5%. However, the electrolyte is poisonous to people and may cause a fire in some extreme conditions. Comparing the load-displacement of the bare cell to the battery cell, as shown in Figure 11 (left), we can draw a conclusion that the shell casing can provide the bare cell with much protection when facing the mechanical load. Finally, the load-displacement curve of the pouch cells in Figure 11 (right) studied by Sahraei [4] didn’t show a suddenly increasing stage like prismatic, which means the aluminum shell casing of the prismatic battery can contribute more than the laminated aluminum film of the pouch cells.

Indentation of Bare Cells and Battery Cells by a Hemispherical Punch

For this experiment, the radius of the hemispherical punch was \( R = 7.5 \text{mm} \), which is comparable to the half thickness of the cell. It is thought that such geometry represents a realistic scenario of a foreign-object intrusion into a battery. The hemispherical punch speed is 1mm/min, as shown in Figure 12 and Figure 13. The measured load-displacement relation for bare cells and battery cells is shown in Figure 14. Unlike the plate compression condition, the load-displacement curve is little different between the shell cell and bare cell expect the peak force. There is not a significant platform stage of local indentation test on cell and bare cell, but the force drops at 6.18mm point. From the view of voltage and temperature, shown in Figure 15, the drop of voltage and rise of temperature at 373 second indicated the internal short circuit of the battery cell. The displacement of the voltage changing point is 6.20 mm which is closely to the peak load displacement in Figure 14.
As known in section 2, the structure of the interior cell is layers stacked electrodes, so the drop of the force may due to the fracture of the layered structure. In order to learn more details about the fracture of the interior cell, the electrodes were disassembled, shown in Figure 16. There were 17 layers of positive electrodes, 18 layers of negative electrodes, and 35 layers separators fractured at the end of the experiment. So the conclusion is that the fracture of multi-layered electrodes and separators caused the internal short circuit of the cell. However, only when the deformation reaches a certain value, the short circuit would occur. But before the short circuit occurs, one or more layers may fracture and lead to micro short circuit which isn’t detected. Actually, a small deformation due to the ground impact on battery pack may cause a micro short circuit, and it would gradually expand to lead to real short circuit, which is an extreme case in vehicle. Micro short circuit will be studied in future.
Compressible foam was shown in the literature to describe the basic properties of the bare cell [6-8]. As a view of Sahrael, the interior of the cell can be treated as a homogenous and isotropic continuum. Because most part of the interior cell (Cu and Al current collectors, graphite and lithium metal oxide powders with a binder) are isotropic, except the polymeric separator which is a small portion of the volume of the cell. The interior material of the prismatic cell is similar to the cylindrical and pouch cell, so from the material point of view, the assumption of isotropy is justified. According to the reference [6], a conceptual graph of the interior cell stress-strain relation is shown in Figure 17. Where $\sigma_i$ denotes the principal stress, $\varepsilon_v$ is the volumetric strain, $Y_c$ is yield stress in compression, $Y_t$ is tensile cut off value in tension, and $E$ is the effective elastic modulus, which is equal to the maximum slope of the stress-strain curve. In this paper, $E=350\text{MPa}$, shown in Figure 6 (right).

A finite element model was developed using the LS-Dyna 971 software. The bare cell was modeled using fully integrated solid elements and the aluminum shell casing is modeled by shell element. All the solid elements were 2mm cubes, and shell elements are 2mm square. The thickness of the shell elements is the initial thickness of the shell casing. There are total 14481 and 13097 elements in flat plate compression model and hemispherical indentation model. As mentioned before, assuming that the interior of the battery cell is homogenous isotropic material, so the model of the actual structure is simplified to be homogenous material, shown as Figure 18. The finite element model is shown in Figure 19.
Mat_63 is a typical model for compressible foam material in LS-Dyna, so it’s chosen to model the interior cell of the battery cell. The stress-strain curve (see Figure 6 (right)) calibrated from the flat plate compression test on the bare cell was used as input for the volumetric strain hardening functions, to control compression properties of the cells. The other parameters are shown in Table 1. A contact-entity of each contact surface is set to “surface to surface” type. The friction coefficient and scale factor slide interface penalties have a great influence on simulation result. Based on experience, the friction coefficient is set to 0.3 and the scale factor slide interface penalties is adjusted to 0.22, which can obtain a good correlation to the test as shown in Figure 20 and Figure 21, that proved the assumption of homogenous isotropic material for bare cell is feasible.

Table 1. Parameters of the finite element model.

<table>
<thead>
<tr>
<th>Part</th>
<th>Material</th>
<th>Density (kg·m⁻³)</th>
<th>Elastic modulus (GPa)</th>
<th>Poisson ratio</th>
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<tbody>
<tr>
<td>Shell casing</td>
<td>(#MAT_24)</td>
<td>2700</td>
<td>69</td>
<td>0.30</td>
</tr>
<tr>
<td>Inner cell</td>
<td>(#MAT_63)</td>
<td>2000</td>
<td>0.35</td>
<td>0.01</td>
</tr>
<tr>
<td>Plate / Punch</td>
<td>(#MAT_21)</td>
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<td>210</td>
<td>0.30</td>
</tr>
<tr>
<td>Sustaining plate</td>
<td>(#MAT_1)</td>
<td>7800</td>
<td>210</td>
<td>0.30</td>
</tr>
</tbody>
</table>

Figure 19. Finite element modeling of flat compression (left) and punch indentation (right).

Figure 20. Comparison of test and simulation for battery cell hemispherical punch.

Figure 21. Comparison of test and simulation for battery cell hemispherical punch.
Discussion and Conclusions

(1) Flat plate compression on prismatic lithium-ion bare cells help to understand the mechanical behavior of the interior material and engineering stress-strain curve of prismatic lithium-ion cells, which is similar to cylindrical and pouch bare cell. But the aluminum shell casing of prismatic cell can provide more protection than Al-plastic film of the pouch cell. Flat plate compression on prismatic lithium-ion cells didn’t cause the fracture of the bare cell, but the shell casing cracked and electrolyte were squeezed out which may lead to a fire So the design of aluminum shell casing should consider both mechanical strength and specific energy for lightweight.

(2) Hemispherical punch indentation tests were also performed on the cells. Load, displacement temperature and voltage were recorded to determine the internal short circuit under local mechanical loading. The drop of the force and voltage indicate the internal short circuit and may lead to thermal runaway. Compared to flat plate compression, the local indentation deformation is more common in vehicle crash or ground impact. From the result of experiment, the little local deformation on the shell casing may cause fracture of the stacked layers before the drop of force and voltage, which may cause a micro short circuit in the cell without detection. Local indentation is widely meet in vehicle crash, so it is important to design a good structure to protect safety of the battery cells in a running vehicle.

(3) Using the engineering stress-strain curve and elastic modulus to develop the FE model can correctly predict the mechanical behavior of the prismatic cells. Moreover, the simulation results proved that the homogenous isotropic compressible material can be used to model the inner cell of the battery cell. Additionally, conclusion in this paper shows that the simplified homogenous material model is applicable to a variety of batteries under compression loading, including cylindrical, pouch and prismatic cells, but needed to change in some other conditions like tensile or shearing. Although this model is not perfect, it can prove that the assumption of inner cell to homogenous isotropic is justified and MAT_63 compressible material can be used to model the compressive properties of the cells. From the viewpoint of safety design to develop a more precise finite element model is urgent need on electric vehicle battery system safety designing.

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References


