

Review

Safety Performance and Failure Criteria of Lithium-Ion Batteries under Mechanical Abuse

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Abstract: With the increasing global focus on environmental issues, controlling carbon dioxide emissions has become an important global agenda. In this context, the development of new energy vehicles, such as electric vehicles, is flourishing. However, as a crucial power source for electric vehicles, the safety performance of lithium-ion batteries under mechanical abuse has drawn widespread attention. Evaluating the safety performance of lithium-ion batteries requires in-depth research. This paper provides a review of recent experimental and numerical simulation studies on the mechanical abuse of lithium-ion batteries. It showcases the main methods and conclusions of experimental research, compares different response forms under quasi-static and dynamic loading, discusses the causes of strain-rate dependence in lithium-ion batteries, and briefly describes the impact of the state of charge (SOC) on safety performance under mechanical abuse, as well as the influence of mechanical abuse on battery capacity and impedance characteristics. Furthermore, this paper summarizes the methods of numerical simulation research, analyzes the advantages and disadvantages of detailed modeling and homogenized modeling methods, summarizes the strain-based internal short circuit failure criteria, and reviews numerical predictive models based on multiphysics coupling. Finally, it presents the latest progress in studying the safety performance of battery packs through numerical simulations.



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1. Introduction

Lithium-ion batteries are widely used in electric vehicles due to their high energy density and cycling efficiency [1]. With the improvement of battery technology, increased energy density, and reduced production costs, major automobile manufacturers are actively introducing the next generation of electric vehicles [2]. Electric vehicles (EVs) have experienced strong growth worldwide, according to the International Energy Agency's (IEA) "Global Electric Vehicle Outlook 2023" report. The report highlights that the EV market is undergoing exponential growth, with sales surpassing 10 million vehicles in 2022. In the first quarter of 2023 alone, over 2.3 million EVs were sold, and it is projected that global sales will increase by 35% in 2023, reaching 14 million vehicles. This will result in EVs capturing an 18% share of the overall automotive market [3]. By 2026, global demand for lithium-ion batteries is expected to reach 1156 GWh, primarily driven by the significant demand from the electric vehicle sector, which represents an \$860 billion market [4]. Despite the remarkable growth of electric vehicles, the safety of batteries remains a critical issue that demands urgent research attention.

Lithium batteries are divided according to the positive electrode material system. The current positive electrode materials include lithium cobaltate (LCO), lithium manganate (LMO), lithium iron phosphate (LFP), ternary materials (lithium nickel-cobalt manganate

(NCM) and lithium nickel-cobalt aluminate (NCA)) and others. These compounds provide sites for the insertion and extraction of lithium ions, enabling the charge and discharge process of the battery. The negative electrode material is primarily graphite, which can intercalate and release lithium ions. The commonly used electrolyte in lithium-ion batteries is an organic solution, typically an organic carbonate solvent containing lithium salt, such as LiPF₆. The electrolyte facilitates the conduction of lithium ions, enabling ion exchange between the positive and negative electrodes. The separator in a lithium-ion battery is usually made of polymer material, which prevents direct contact between the positive and negative electrodes, prevents short circuits, and allows for the transport of lithium ions. Such a structure and materials enable lithium-ion batteries to have high energy density but also pose certain usage risks.

This is particularly due to the inherent structural characteristics of lithium-ion batteries, which pose a risk of internal short circuit (ISC) and subsequent thermal runaway in the event of a collision. This risk has garnered significant public attention and has been the subject of extensive research in the academic community [5]. While the failure of automotive lithium-ion batteries results in the propagation of abnormal heat within the battery pack, leading to fires, it is important to examine the triggering factors of thermal runaway. Often, these factors arise when the battery's structure is subjected to mechanical abuse that exceeds its tolerance, causing abnormal changes in the battery's electrochemical processes and generating significant heat. Therefore, research on battery safety must carefully consider the mechanical response of batteries under conditions of mechanical abuse.

Extensive research has been conducted on the safety issues of batteries under mechanical abuse. Zhang et al. provided a comprehensive overview of the thermal safety concerns associated with lithium-ion batteries [6]. They conducted tests and modeling on the thermal behavior and thermal runaway of battery cells, as well as investigated thermal management strategies for battery packs. Deng et al. further examined and researched the modeling and testing methods for studying battery safety performance under mechanical abuse [7]. Liu et al. provided a description of the battery response under mechanical abuse from the perspectives of mechanics, electrochemistry, and thermodynamics by reviewing the evolution process. They addressed the battery response issues under multi-physics field coupling through theoretical analysis, experimental investigations, and modeling. The new modeling methods proposed by them can offer useful guidelines for the design, safety assessment, and testing of lithium-ion batteries [8]. Feng et al. discussed the safety issues of lithium-ion batteries under various abuse conditions, including mechanical abuse, electrical abuse, and thermal abuse. They proposed the concept of a three-tier protection system to mitigate the hazards of thermal runaway and enhance prevention and early warning of thermal runaway incidents [9]. Wang et al. conducted a comprehensive review of case studies on thermal runaway incidents in lithium-ion batteries. They discussed potential measures for fire prevention in lithium-ion batteries [10]. Xue et al. studied the tensile strength, elastic modulus, and fracture modes of separators under uniaxial tension at different loading angles and with linear notches [11]. Moreover, the cost of the Traction Current Source (TCS) for electric vehicles accounts for around 40% of the overall vehicle cost. Therefore, it is crucial to conduct research on the performance and lifespan of batteries after experiencing impacts [2]. Yang et al. proposed a deep Gaussian process regression (DGPR) method for state of health (SOH) estimation of lithium-ion batteries, based on Gaussian processes and deep networks. This method provides a reliable basis for the health management of lithium-ion batteries [12]. Li et al. proposed an aging feature extraction method based on electrochemical models to capture the aging mechanism of batteries. This method effectively improves the accuracy of state of health (SOH) estimation under different application scenarios and battery charge-discharge modes [1]. Shchurov et al. provided an overview and comparative analysis of various types of batteries, including the most modern lithium-ion batteries. They extensively analyzed the causes of degradation and established processes occurring in lithium-ion batteries during charging, discharging, idle, and challenging operating conditions [2].

Despite conducting extensive research, a crucial task for the development of automotive lithium-ion batteries still lies in gaining a deep and comprehensive understanding of the potential safety risks under abusive mechanical conditions, as well as the underlying mechanisms behind their occurrence. Based on this understanding, it is necessary to establish a set of practical and well-defined criteria for determining the failure of lithium-ion batteries. This will enable better design, testing, and evaluation of the safety performance of these batteries.

With the rapid development of artificial intelligence, it has also played a role in the safety performance assessment of lithium-ion batteries. For example, Su et al. have developed a capacity estimation method based on artificial intelligence techniques, which takes into account the actual operating parameters. This method enables adaptive boost charging, allowing for better state estimation and adaptive adjustment of charging strategies during charge and discharge cycles [13]. Liu et al., on the other hand, have conducted research related to battery life diagnosis using artificial intelligence techniques. They have attempted to predict battery life trajectories [4]. Lombardo et al. conducted a comprehensive review of the application of artificial intelligence methods in battery research. Currently, artificial intelligence techniques are being applied in various aspects of battery research, including material design and synthesis, electrode and cell manufacturing, material and electrode structure characterization, battery diagnostics, and lifetime prediction. However, challenges such as the difficulty in accurately representing real-world operating conditions, the shortage of training data, and the lack of unified standards are still obstacles that need to be overcome in the application of artificial intelligence techniques in battery research [14].

This is a rapidly developing subject of highly focused interest. This article tries to summarize the current state of the art of the research and aims to consolidate the knowledge gained on the safety performance of lithium-ion batteries under mechanical abuse conditions, focusing on battery response and failure criteria. The article summarizes common research methods and conclusions. In Section 2, discussion is given on the mechanical response and failure characteristics of lithium-ion batteries under quasi-static and dynamic loading, analyzing the causes of the strain rate dependence on dynamic loading, the influence of State of Charge (SOC) on battery safety performance, and changes in battery capacity and internal resistance under mechanical abuse. In Section 3, the importance of conducting mechanical abuse studies on lithium-ion batteries is highlighted through numerical simulation methods. It compares the advantages and disadvantages of using homogeneous and detailed models in the modeling process, summarizes ISC failure criteria based on the battery strains or deformation, explores ISC behavior prediction based on multi-physics coupling, and discusses battery pack safety performance optimization based on numerical simulation.

2. Mechanical Response and Performance Changes Mechanisms of Lithium-Ion Batteries under Abusive Conditions in Experimental Environments

2.1. Mechanical Response and Failure Characteristics under Different Loading Conditions

Lithium-ion batteries are formed by stacking or winding multiple layers of porous structure, (Figures 1 and 2), pouch batteries are typically composed of multiple layers of materials stacked together, allowing for greater flexibility and versatility, and customization according to specific requirements. In the initial stage of loading, pouch batteries have lower resistance to impact compared to 18650 batteries due to their lack of a rigid metal casing. On the other hand, 18650 batteries are usually formed by winding multiple layers of materials, and they have standardized size requirements. The external metal casing also provides relatively better protection in the initial impact. Lithium-ion batteries often exhibit characteristic evolution processes and changes in material properties when subjected to impact or compression, many studies have summarized the variations of load with displacement based on the force-displacement curve of the battery. For instance, Li et al. identified five stages of load-displacement behavior for cylindrical 18650 batteries under axial compression, including a slow rising stage, rapid rising stage, slight decrease or plateau stage, secondary

rapid rising stage, and rapid decrease stage [15] (Figure 3). Zhu et al. also found that the force-displacement behavior of all batteries followed a trend of “slow rise-rapid rise-slight decline-rapid rise” until a sudden drop in the curve occurred when the battery failed [16]. This process can be summed up in a flowchart as shown in Figure 4. In Zhang et al.’s study, it was found that the force-displacement curve of the battery exhibited an ascending-descending-plateau-ascending pattern under dynamic loading conditions. This pattern differed from the force-displacement curve of the 18650 battery under quasi-static loading. Furthermore, their research also discovered that the occurrence of ISC (internal short circuit) did not necessarily coincide with the force decrease during dynamic loading [17]. While there may be slight variations in the description of force-displacement curve development for batteries under different experimental conditions, the aforementioned study suggests that the observed load changes reflect variations in the mechanical response of batteries due to the evolution of their internal structures. The underlying mechanisms, which have universality, will be further elucidated in the following text.

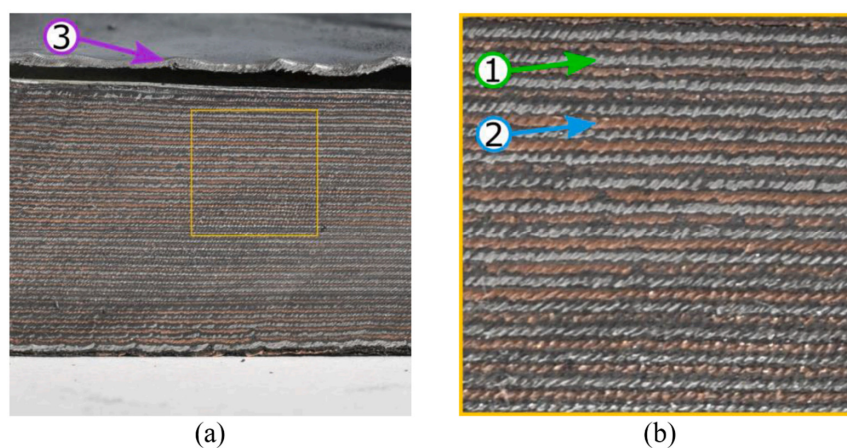


Figure 1. Micrograph of the undeformed structure of the Lithium-ion pouch cell, (a) full height and (b) close up view. ① Cathode with aluminum foil; ② anode with copper foil; ③ soft aluminum pouch [18].

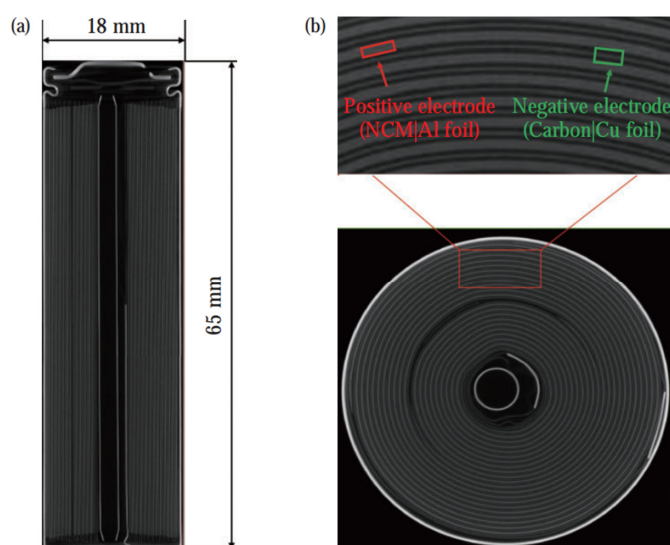


Figure 2. CT image of 18650 lithium-ion battery [15]. (a) Longitudinal cross-sectional view of 18650 battery; (b) schematic of electrode in multilayer winding structure and axial cross-sectional view of 18650 battery.

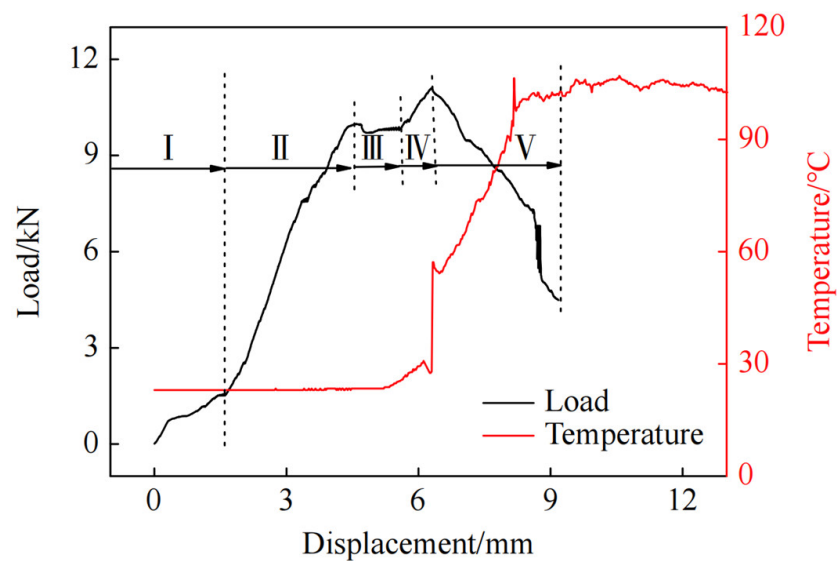


Figure 3. Load temperature-displacement curves of the 100% SOC battery [15].

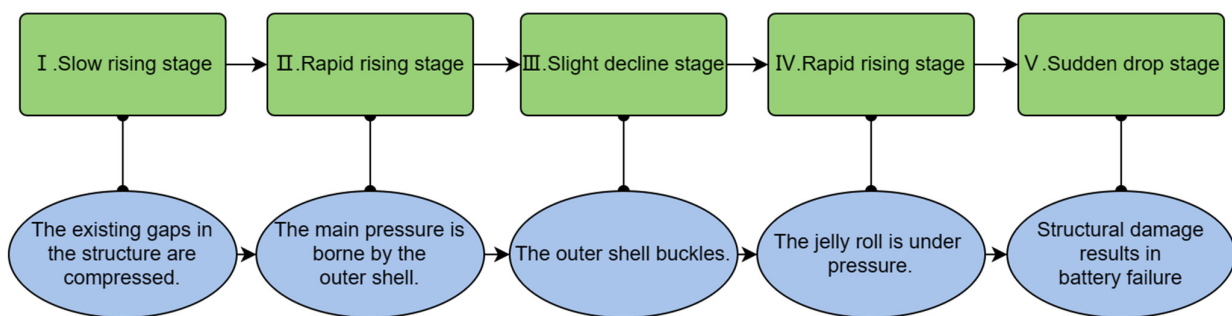


Figure 4. Flow chart and mechanism of load changes at each stage of 18650 battery under axial loading.

Although the actual force-displacement curves of the battery differ under different loading conditions, considering the structural aspect of the battery, being composed of multi-layered porous materials (such as separators) wound or stacked together, it typically undergoes a progression of shell compression, densification, reinforcement, and failure as displacement increases during loading. During the shell compression stage, the load is primarily borne by the metallic shell, which undergoes deformation. As the deformation increases, the core also begins to bear the load. In the densification stage, due to the presence of numerous voids in the porous material, which has lower intrinsic strength and is easily compressed, the displacement increases faster compared to the load. The porosity of the battery continues to decrease, and the nature of the material gradually transitions from foamed material to densified material, as inferred from the concavity or convexity of the force-displacement curve [19] (Figure 5). During the reinforcement stage, the already densified core undergoes further compression leading to plastic deformation. The uneven distribution of stress intensifies, leading to phenomena such as multilayer buckling, radial cracks, collapse and flow of anode and cathode particle coatings, and fracture of the current collector. Ultimately, these conditions result in battery failure characterized by voltage drop and rapid temperature rise due to ISC (internal short circuit) occurrence [20]. It should be noted that in some cases, there can also be delayed failure of the battery. This means that after reaching the peak load, the voltage does not exhibit a sudden drop but rather fluctuates and rebounds to normal levels. However, within a few days after the loading is complete, the battery self-discharges and eventually fails completely. This phenomenon is often attributed to a soft short circuit occurring within the battery [21]. The presence of such delayed failure poses a significant safety hazard for electric vehicles. As the electric

vehicle market continues to expand, it is necessary to conduct systematic research on the delayed failure mode and establish corresponding failure criteria. This would help ensure the safe operation of electric vehicles.

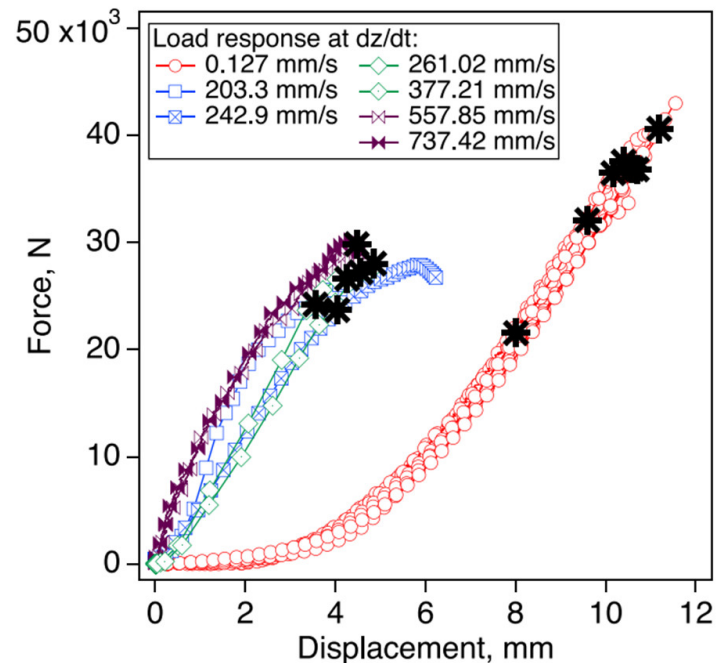


Figure 5. The force-displacement response of battery cell stack varies with the deformation rate [19], and the * indicates battery failure.

From the perspective of loading direction differences, the ultimate displacement of a battery under radial loading is greater than its ultimate displacement under axial loading [22], and the ultimate load that a battery can withstand under radial plate compression is also much greater than its ultimate load under axial compression [15]. This is because under axial loading, each layer of the winding can be considered as a thin-walled cylindrical shell, which is prone to buckling and wrinkling. In contrast, under radial loading, the layers of winding can be viewed as a stacked structure, which is compacted before experiencing collapse. Therefore, the battery has a larger load-carrying capacity under radial loading compared to axial loading. In terms of voltage variation, under axial loading, the battery voltage exhibits a distinct stepped decrease, while under radial plate compression, the battery voltage drops to its lowest value in a single step. In terms of thermal runaway, axial compression tends to result in a milder degree of thermal runaway compared to radial plate compression [15].

The mechanical response of batteries differs significantly between quasi-static loading and dynamic loading conditions. Under quasi-static loading, the ultimate load and ultimate displacement of the battery increase with the loading rate [23] (Figure 6); however, under dynamic loading, the ultimate load and ultimate displacement of the battery tend to decrease gradually with an increasing loading rate [21]. This counterintuitive phenomenon exhibits a significant strain rate dependence. It is worth noting that the strain rate dependence of the battery is relatively small under quasi-static loading, while it becomes more pronounced at higher impact velocities. Therefore, the curve variations in Figure 6 are not very significant, while the curves for different impact velocities in Figure 5 show more noticeable differences. Under quasi-static loading, batteries often experience severe thermal runaway at a high state of charge (SOC). In contrast, under comparable SOC and deformation conditions, batteries subjected to dynamic loading exhibit relatively milder thermal runaway [24].

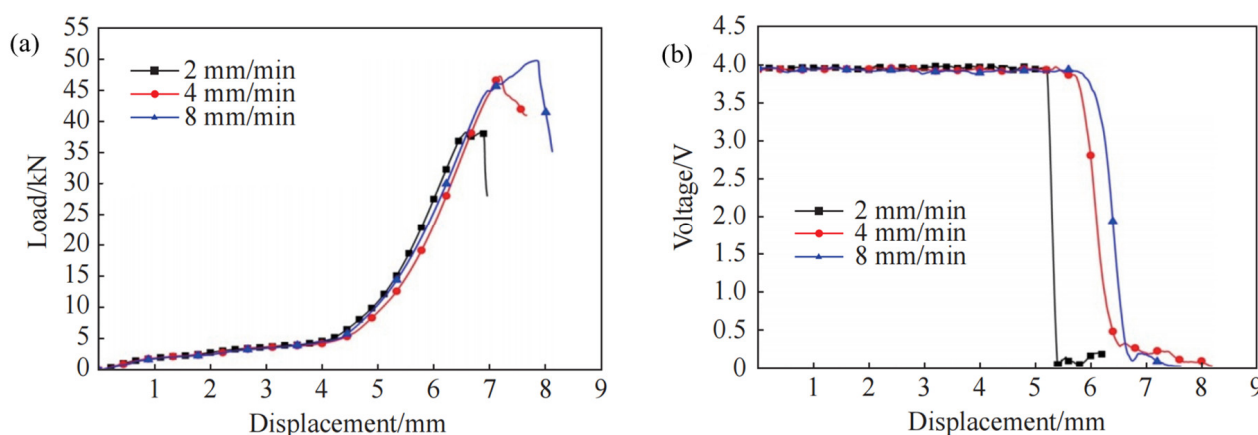


Figure 6. (a) Load-deformation curve of battery at different loading speeds; (b) Voltage-deformation curve of battery at different loading speeds [23].

2.2. Strain Rate Dependency Mechanism Analysis

The strain rate dependency of lithium-ion batteries is manifested as follows: under quasi-static loading, the ultimate load and ultimate displacement of the battery increase with increasing loading rate. However, under dynamic loading, the ultimate load and ultimate displacement of the battery decrease with increasing strain rate [18]. This is because as the strain rate increases, the inertial effects of the material become more apparent, leading to the majority of the impact energy being absorbed by a smaller region at the impact front. This results in more severe local damage, directly leading to membrane rupture and contact between the anode and cathode. The battery's ability to withstand impact is weakened. Different failure mechanisms exist under different strain rates, in their research, Zhang et al. [17] identified two critical velocities. When the loading speed is below 8 m/s, both the inertial effects and stress wave effects of the material are not significant, resulting in relatively uniform deformation of the battery at a global scale. Cracking starts from the center of the winding core, and the failure displacement is approximately 6 mm. When the loading speed is greater than 8 m/s but less than 40 m/s, the stress wave effect dominates the overall mechanical response, leading to cracks in the upper part of the winding core caused by the tensile wave stress superimposed from the concave surface inside the core. The failure displacement in this case is approximately 5 mm. When the loading speed exceeds 40 m/s, the inertial effect becomes dominant, resulting in rapid battery failure due to the enormous energy absorbed by a minuscule region at the loaded end. The failure displacement reduces abruptly to approximately 2 mm. However, it is worth noting that, in dynamic loading, the actual damage area within the battery is relatively small [24]; therefore, thermal runaway in such cases is often not severe or even does not occur, which is significantly different from the thermal runaway mode observed under quasi-static loading conditions.

The strain rate dependency is directly related to the structure of porous materials with loosened membranes. Li et al. demonstrated through their study on a porous honeycomb material that it exhibits significant strain rate dependency [25]. As the strain rate increases, the compressive strength and elastic modulus of the material also significantly enhance. For membranes composed of porous honeycomb materials, they play a crucial role in the dynamic impact process on the winding core. On the other hand, it is precisely because the loose and porous structure itself has good energy absorption capabilities that more energy is localized and accumulated in the impacted area due to the inertial effects. However, an increasing amount of research suggests that the loose and porous structure of the membrane not only contributes to the strain rate effects in dynamic loading on a single solid phase but also, from a fluid-solid coupled perspective, the viscous effects generated by the rapid flow of liquid electrolyte in the pores of the membrane are important factors causing strain rate dependency. Research has shown significant differences in the

compressibility [26] and resistance [27] of liquid electrolytes under quasi-static and dynamic loading conditions, because the application of external loads creates stress fields inside the battery, and the liquid electrolyte flows within the pores along stress gradients caused by these stress fields. The viscosity resistance of the liquid during the flow process is highly dependent on its flow velocity. Zhu et al. [27] conducted a study on this and, based on the mechanism of liquid viscosity dissipation, developed an analytical model for the dynamic stiffening effect in battery structures. They demonstrated that the strain rate dependency in wet batteries containing electrolytes is significantly stronger than in dry batteries without electrolytes (Figure 7a,b); indeed, they also demonstrated that there is a correlation between the viscosity resistance of the electrolyte fluid and its flow velocity. This correlation provided an explanation for the strain rate effect in dynamically loaded lithium-ion batteries. They also derived a theoretical formula for the average stress experienced by wet batteries under impact, which can be expressed as:

$$\sigma_{avg}(\varepsilon_v) = \frac{1}{\pi r_0^2} P(\delta) = A \varepsilon_v^n + \frac{\pi r_0^2 \mu v_p}{8 H_0 (1 - \varepsilon_v)} \frac{150}{\Phi_s^2 D_p^2} \frac{(1 - \phi_0 + \varepsilon_v)^2}{(\phi_0 - \varepsilon_v)^3} \quad (1)$$

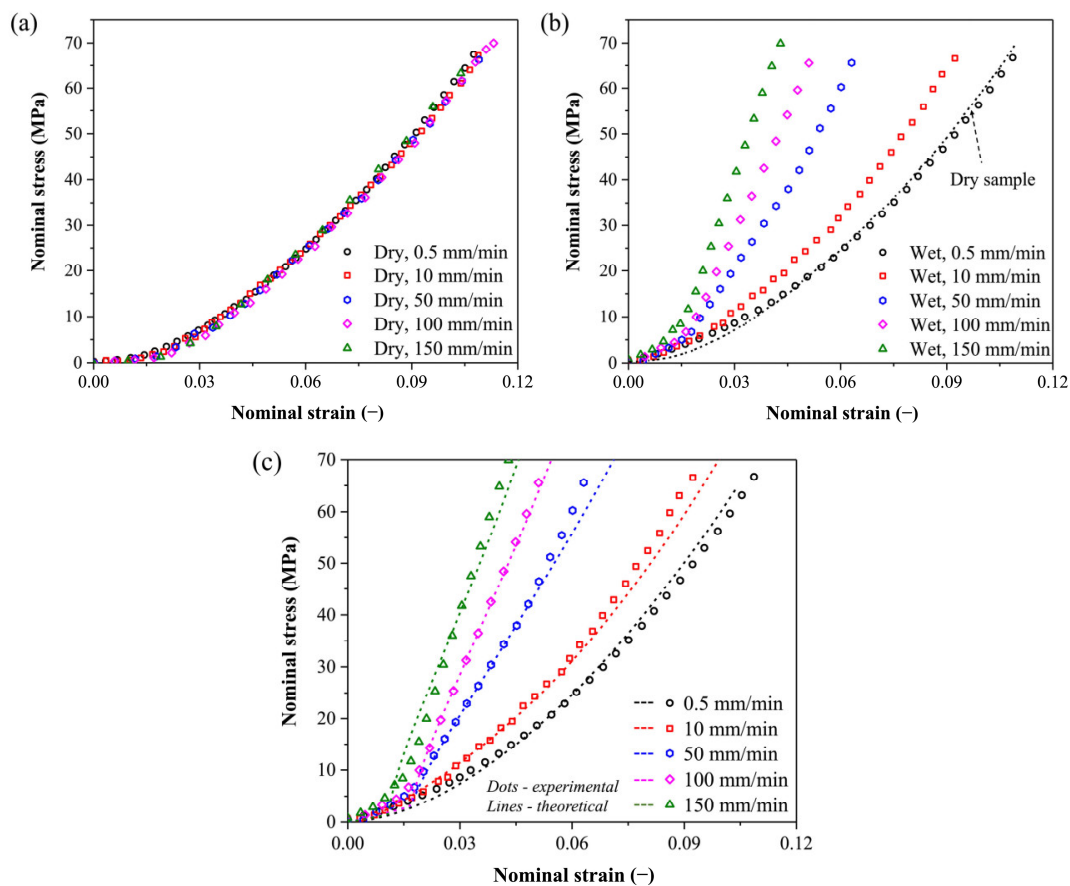


Figure 7. Experimental results and theoretical predictions. (a) Nominal stress–strain curves of dry square samples cut from the battery cell; (b) nominal stress–strain curves of wet square samples cut from the battery cell; (c) prediction of the theoretical model vs. experimental results showing almost a perfect correlation [27].

Although this formula is quite complex, it shows a good fit with experimental results (Figure 7c).

In their study, Kalnaus et al. [19] also pointed out that the transformation of material properties, known as the strain rate effect, can be explained by the influence of liquid electrolyte filling in the electrode and separator pores. In studies [28,29], it has been observed that the fillable separator membranes exhibit significant hardening under impact loads. The

results indicate that the pore elastic effect of the liquid becomes more evident at strain rates of 10 to 31 /s and higher. In this case, the compressive response is determined by the rate at which the liquid is squeezed out from the pores which, in turn, is governed by Darcy's Law, Darcy's law states that the fluid velocity is proportional to the pressure gradient as $\epsilon \cdot \vec{u} = -\kappa/\mu \Delta p$ (with ϵ and κ being the porosity and permeability of the solid matrix, and μ the dynamic viscosity of the liquid). In the study conducted by Raffler et al. [30], they found that by using high-speed cameras to observe the surface of batteries under dynamic loading, a noticeable fluid-like behavior was observed on the surface of pouch cells after contact with the impactor. A wave-like shape appeared beneath the packaging of the battery.

2.3. The Impact of State of Charge (SOC) on the Mechanical Response and Safety of Batteries

For safety reasons, the majority of mechanical abuse experiments on lithium-ion batteries are currently conducted at a low state of charge (SOC). However, there are also some studies in the academic community that have been conducted at higher SOC states [15,23,26,31–34] (Figure 8). According to the experimental results from ref. [15], as the SOC increases, there is a slightly noticeable increase in the maximum load that the battery can withstand (Figure 9). In ref. [8], it is noted that during the charging process of batteries, the expansion of the anode can lead to internal stress and result in increased stiffness of the battery [32]. Refs. [35–37] also indicate that batteries with higher SOC exhibit increased stiffness. The research by Chen et al. demonstrates that after charging, the battery core expands, resulting in a change in stress that causes the steel shell to be stretched, leading to the phenomenon of increased battery stiffness [38]. Zhao et al.'s research reveals different hardness variations of Cu current collectors and Al current collectors during cyclic charge-discharge processes [39].

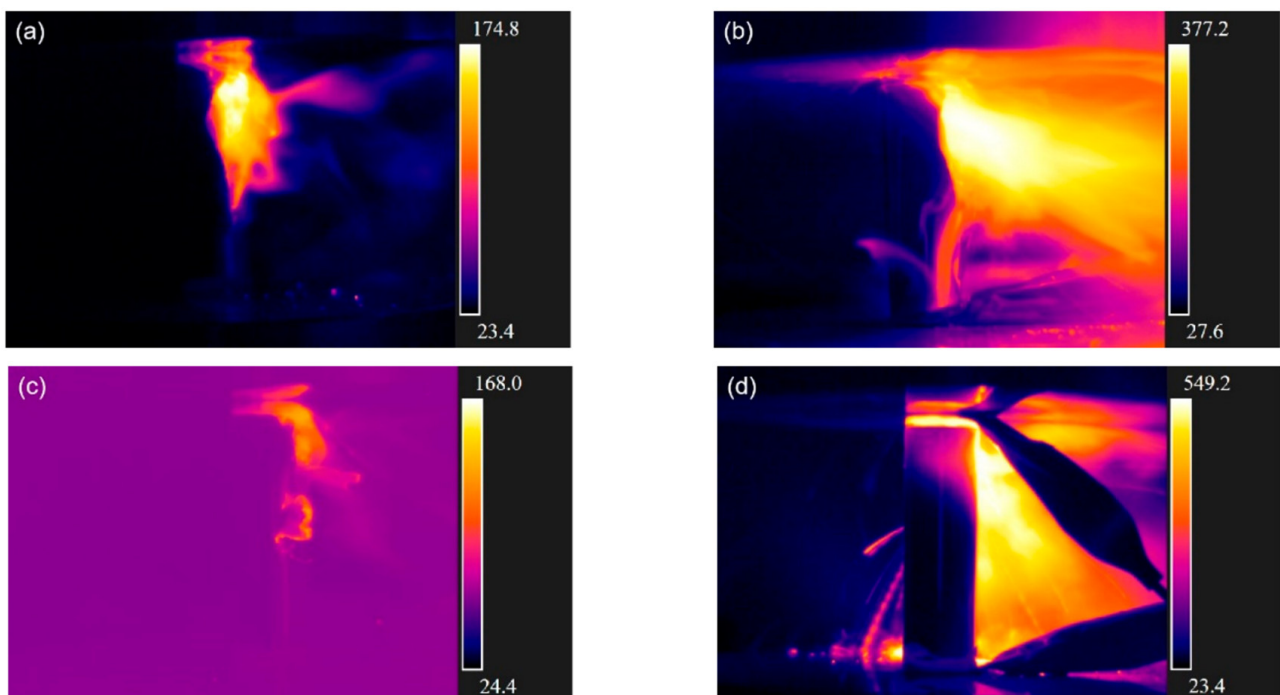


Figure 8. Temperature nephogram under thermal runaway: (a) battery with 40% SOC at 2 mm/min; (b) battery with 40% SOC at 8 mm/min; (c) battery with 60% SOC at 2 mm/min; (d) battery with 60% SOC at 8 mm/min [34].

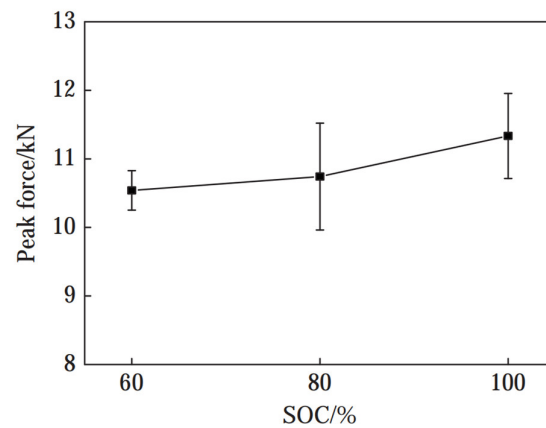


Figure 9. Peak force of batteries with different SOC levels [15].

In ref. [28], Cannarella et al. state that batteries with high SOC are unstable and more prone to voltage drop under mechanical abuse. Wang et al.'s experimental results indicate that batteries with high SOC are more susceptible to thermal runaway under equivalent deformation conditions [15,22,34] (Figure 10). Batteries with high SOC exhibit a faster rate of temperature increase when subjected to mechanical abuse, and this is due to the fact that batteries with high SOC also generate higher currents after experiencing mechanical abuse, resulting in the release of larger amounts of heat [37]. Ren et al. also pointed out in the literature [40] that for batteries with a low state of charge (SOC), the heat generated during the internal short circuit (ISC) is smaller and the chemical reactions inside the battery are still controllable. However, for batteries with high SOC, a large amount of heat is released due to ISC, causing the battery temperature to rapidly rise to the triggering temperature for SEI membrane decomposition and anode decomposition. This leads to the rupture and explosion of the battery casing due to the generation of a large amount of gas during decomposition. The accumulation of abnormal heat can further generate more heat, resulting in a vicious cycle and being an important mechanism for thermal runaway in high SOC batteries [24,41,42].

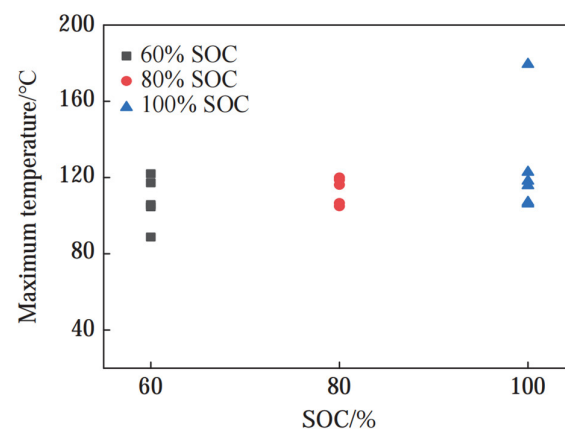


Figure 10. Maximum temperature of batteries with different SOC levels [15].

2.4. The Evolution of Battery Capacity and Impedance Characteristics under Mechanical Abuse

For batteries that have undergone mechanical abuse but have not failed, determining the changes in their capacity and impedance characteristics holds economic significance and practical value. Wang et al. [22] found that the greater the deformation of a battery, the faster its capacity decreases during charging cycles (Figure 11), this change can be understood from the perspective of the electrode's porous structure. When the electrode is compressed, the pores experience a certain degree of closure, resulting in a decrease

in the passage rate of lithium ions and impacting the battery's capacity. In the study by Xi et al. [43], it was also found that under dynamic loading, the resistance of the battery increases. This phenomenon has also been observed in studies [27,44].

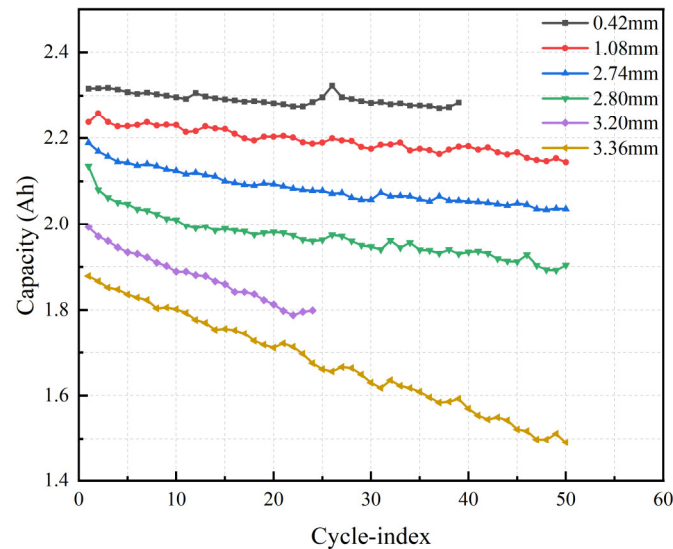


Figure 11. Capacity decay curves of batteries with 6 different residual deformations [22].

2.5. Current Experimental Characterization Faces Certain Challenges/Issues

In-situ characterization of the actual operational processes of batteries has always been a goal pursued by the academic community. Wei et al. achieved this goal by utilizing Raman spectroscopy to detect lithium ion concentration in the liquid electrolyte on the surface of optically transparent lithium-ion battery cathode particles [45]. Samajdar et al. utilized in-situ vibrational spectroscopy to dynamically investigate the structure and chemical changes at the electrode-electrolyte interface under battery cycling conditions [46]. Chen et al. developed an in-situ measurement method for detecting winding core mechanical pressure by utilizing embedded thin-film flexible pressure sensors. This method can be used to assess the mechanical response of the winding core after long-term operation [47]. However, batteries are essentially closed systems, making it challenging to directly observe internal processes such as chemical reactions, ion transport, and electron conduction. The difficulty in in-situ characterization of batteries lies in finding non-destructive ways to observe these processes comprehensively. Additionally, lithium-ion batteries are complex physical-chemical systems with multiple coupling fields. Therefore, analyzing their operating mechanisms requires a comprehensive and detailed observation of the relevant information regarding mechanics, electrochemistry, and thermal processes. This information includes material stiffness and deformation, electrochemical reaction rates and heat generation, heat transfer within the battery and battery pack, phase transitions, and material transport efficiency. However, achieving such comprehensive observations poses high demands on researchers' observational capabilities and associated costs.

Conducting physical research on batteries faces challenges such as the difficulty of obtaining comprehensive control over key information, high economic costs, and inadequate safety. Particularly in experiments that involve mechanical abuse of battery samples to study their mechanical response, the reusability of battery samples is extremely low, and there are inherent safety risks involved. This often limits the scale of physical experiments, and there are relatively fewer experiments conducted at a high state of charge (SOC) due to safety concerns. These factors hinder further research on battery operation mechanisms and response mechanisms. Therefore, in the following chapters, this article will further discuss the progress made in research using numerical simulation methods.

3. Numerical Simulation Methods and Failure Criteria for Mechanical Abuse of Lithium-Ion Batteries

3.1. Comparison between Homogenized Models and Detailed Models for Batteries

Taking cylindrical batteries as an example, they are mainly composed of components such as a metal casing, separator, and electrodes. Although the metal casing plays a significant role in bearing mechanical abuse, its material and structure are relatively uniform, making the mechanical response of the metal casing under mechanical abuse clear and straightforward. On the other hand, the cell core structure of the battery is more complex, as it consists of layers of positive electrode-separator-negative electrode-separator that are stacked and wound together (Figure 12), both the complexity of the constituent materials and the structure make numerical simulation of the cell core part more challenging. At the same time, some literature indicates that the mechanical response of the cell core plays a significant role in the overall response of the battery under mechanical abuse [48,49].

The construction of models directly relates to the accuracy of mechanical, electrochemical, and thermal responses of battery cells under mechanical abuse, as well as the computational difficulty of conducting simulations. Kumaresan proposed a thermal model for lithium-ion batteries, which was used to predict the discharge performance at different operating temperatures [50]. Domenico et al. conducted numerical computations on the spatial evolution of solid concentration in the two electrodes of lithium-ion batteries. They performed three-dimensional finite element simulations on cylindrical battery cells and investigated the performance of battery cells under various loading conditions [51]. Avdeev et al. developed and compared two homogenization methods for modeling the cell core in cylindrical lithium-ion batteries. They proposed a novel one-dimensional electrode model for lithium-ion batteries, which for the first time considered the electrochemical coupling among particles with a realistic size distribution obtained from tomography imaging data [52]. If a simple block material or rigid body is used to model the module, it may result in the loss of computational accuracy. To address this crucial engineering issue, Tang et al. proposed a general method for establishing a homogenized model to compute cylindrical battery modules [53]. Muresanu et al. proposed a homogenized finite element model for a battery cell and validated it through experimental tests on individual materials and impact tests on the entire battery [54]. The model developed by Chen et al. accurately considers the layered structure of the battery stack, enabling a comprehensive and detailed simulation of the operating conditions of the battery and battery pack [55]. Wang et al. were the first to establish a refined model for the ISC triggering mechanism in commercially available 18650 cylindrical batteries, which describes the deformation of the individual cell [56]. Shekar et al. proposed a novel real-time State of Charge (SOC) estimation method for lithium-ion batteries by applying the Particle Swarm Optimization (PSO) algorithm, a bio-inspired optimization method, to a refined electrochemical model of an individual cell [57].

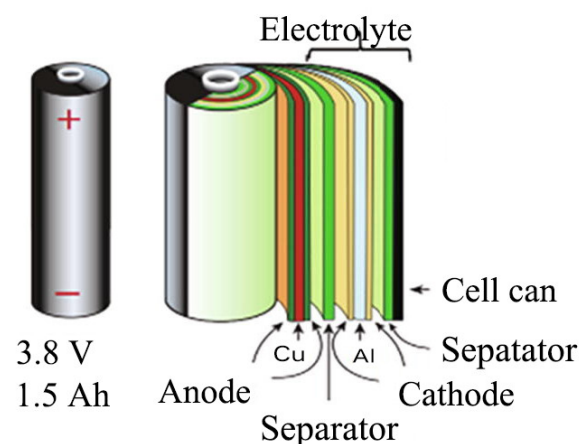


Figure 12. Repeatability unit (RVE) of a lithium-ion battery, and cross-sections of the components [58].

The use of a refined model allows for highly accurate calculations of the mechanical response of the winding core under mechanical abuse. However, the multi-layer winding structure of the core significantly increases the number of grids in the detailed model, leading to a significant reduction in simulation efficiency (Figure 13). This is particularly evident in impact and collision simulations of battery packs or vehicles, where a large number of batteries and the coupling of multiple physical fields contribute to excessively high simulation costs.

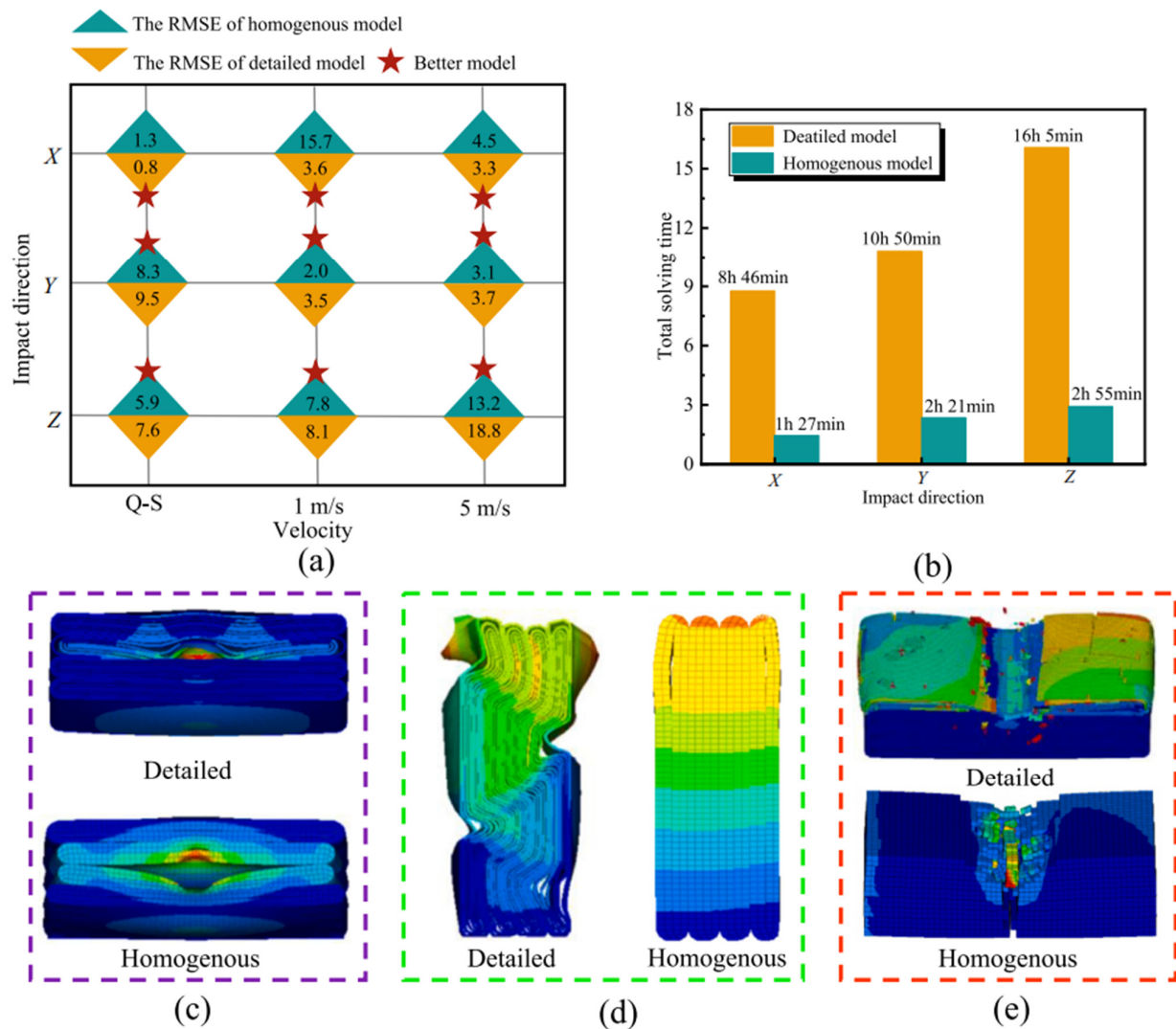


Figure 13. The comparison on prediction accuracy and efficiency of detailed and homogenous models as well as failure behavior of jellyrolls, (a) The RMSE of homogenous and detailed models; (b) The total solving time of homogenous and detailed models; (c) The failure behavior of jellyrolls in the X direction; (d) The failure behavior of jellyrolls in the Y direction; (e) The failure behavior of jellyrolls in the Z direction [59]. From (c–e), it can be observed that the detailed models exhibits higher predictive accuracy compared to the homogeneous models, particularly evident in (c). Due to the excessive single-layer thickness of the homogeneous model, deformation is challenging to be accurately simulated, which is also reflected in (d).

Furthermore, some comparative studies have shown that the simulation accuracy of a refined model may not be higher than that of a homogeneous model at different stages of the same loading process. The authors did not provide an explicit explanation for this phenomenon. However, in reality, in order to establish a refined model that closely matches reality, it is necessary to define the constitutive relationships and material parameters of the

separator, electrodes, current collectors, and even electrolyte in a meticulous and accurate manner. Otherwise, if there are errors in the imposed constraints, excessive constraints can actually lead to a further deviation of the model from real-world conditions.

Using a homogeneous model to simulate the operating conditions of the winding core under mechanical abuse can significantly reduce computational costs. However, the predictive accuracy of the homogeneous model is often inferior to that of the refined model. Research [59] has indicated that this is because the homogeneous model treats the winding core as a single, unified structure, which results in a layer thickness for the core that is much greater than the thickness of individual layers in the refined model. As a result, the homogeneous model is more resistant to bending, leading to greater simulation errors. The detailed and homogeneous model can be seen in Figure 14.

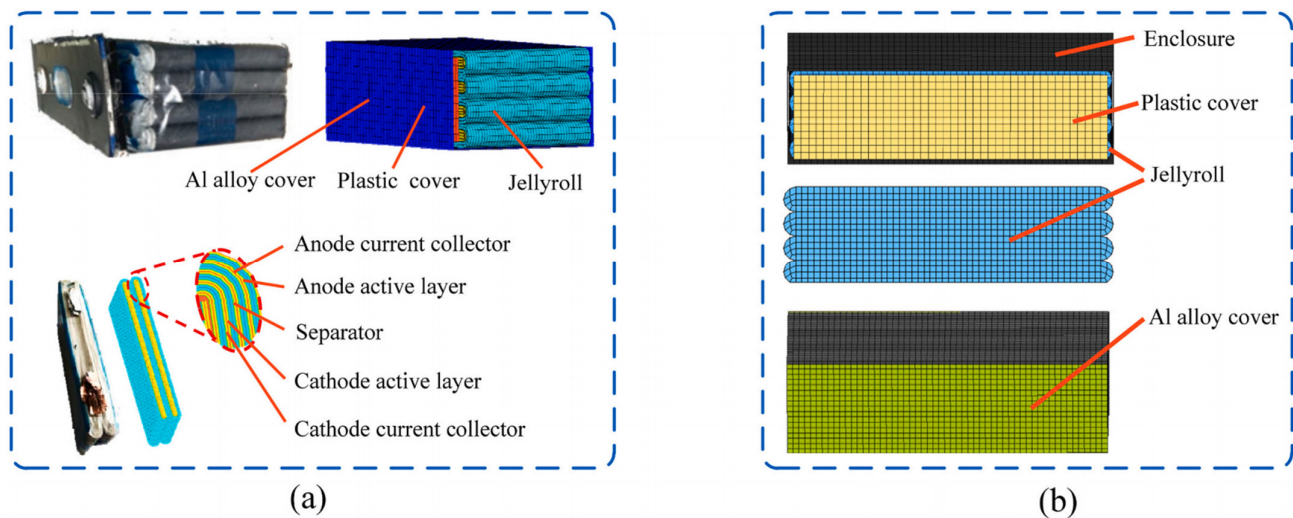


Figure 14. The detailed and homogenous models of battery. (a) Detailed model; (b) Homogenous model [59].

In order to resolve this contradiction, one approach is to appropriately simplify the refined model without significantly reducing simulation accuracy. In some studies, the materials in the refined model are assumed to be isotropic, which reduces computational costs in terms of constitutive relationships. Additionally, in most refined models, the current collector interfaces with the anode and cathode are set as Coulomb friction interfaces, further reducing computational burden [56]. On the other hand, it should make trade-offs according to different problems. For example, in problems involving multi-physics coupling, when the researchers need to accurately determine the location of a short circuit, it is necessary to calculate and understand the global strains, resistances, currents, and temperatures, as well as the failures of critical components. In such cases, the researchers often use refined models for simulation. However, in some more macroscopic problems like collision simulations of battery packs or vehicles, homogeneous models can be used. This is because components such as separators and electrodes in batteries are very small, and their influence on the overall mechanical response prediction is limited. The computational cost savings achieved by using homogeneous models far outweigh the accuracy loss incurred by abandoning refined models [60].

3.2. Establishing a Quantitative Relationship between Battery Strain and Short-Circuit Current (ISC)

In practical operating conditions, the failure of batteries under mechanical abuse is the result of the combined effect of multiple physical fields. Currently, there are numerous studies on failure phenomena, and different researchers have observed and studied the characteristics of these phenomena from different perspectives. Most of the early-established

models often used elastic deformation constitutive relationships, which cannot effectively characterize fracture phenomena, in ref. [61], for the first time, the classical Coulomb and Mohr stress fracture criteria were combined with a uniform isotropic model of cylindrical batteries to associate the jelly-roll failure with internal short circuits, There is also ref. [62] that considers peak stress as a criterion for failure. However, this criterion is not accurate enough under three-point bending and plate compression conditions.

Cheng et al. proposed a failure criterion based on tensile stress, where a spherical indenter is used to induce cracks in the electrode [63]. Sahraei reported experimental and numerical research results on the material failure of electrode components in lithium-ion batteries under mechanical abuse. They developed a finite element model for prediction and applied the maximum strain criterion for determining short circuit failure [64]. Zhang et al. discovered two different mechanisms for the generation of internal short circuits (ISC), thereby elucidating the reasons for the differences in ISC occurrence under different deformation modes [65]. Kermani et al. proposed a method based on experimental results for predicting the mechanical response and failure modes of lithium-ion batteries under dynamic loads [66]. Among various indicators, stress/strain can be considered a key indicator for determining battery failure under mechanical abuse [8]. It should be noted that the failure threshold of the battery is closely related to the State of Charge (SOC). Therefore, even when using strain as the criterion for failure, different failure strains correspond to different SOC levels.

Ref. [67] revealed a quantitative relationship between battery deformation and the occurrence of Internal Short Circuits (ISC). This study utilized experimental data from [68] reported battery samples to validate the established numerical model by examining the corresponding membrane resistance values for four types of contact-induced Internal Short Circuit (ISC) failure modes: anode active material-cathode active material, anode active material-cathode current collector, anode current collector-cathode active material, and anode current collector-cathode current collector, subsequently, using this model, the corresponding relationship between the equivalent plastic strain (PEEQ) and two types of short-circuit modes caused by membrane failure (secondary ISC) and current collector fracture (primary ISC) was established. The critical values of equivalent plastic strain were determined as $\bar{\epsilon}_{eq,minor} = 0.2119$ for the secondary short-circuit mode and $\bar{\epsilon}_{eq,major} = 0.3280$ for the primary short-circuit mode. This study has to some extent clarified the relationship between deformation and ISC, but there are still two issues when using deformation or strain as a criterion for failure and guiding the assessment of faulty batteries in practical applications. Firstly, the relationship between PEEQ and the depth of penetration in different operating conditions is inconsistent, making it challenging to directly use easily measurable data, such as penetration depth, for rapid assessment of battery state. Secondly, this study relied on simulation methods to track the overall condition of the battery, and the value of PEEQ was directly calculated by the simulation program, making it difficult to obtain accurate PEEQ values in real-world applications due to the lack of sufficient parameters for calculation.

3.3. Strain-Based ISC Prediction Considering Multi-Physics Field Coupling

When a battery is subjected to mechanical abuse, it undergoes structural changes. During the loading process, the battery, which initially exhibits loose and porous structural characteristics, goes through a densification-strengthening phase. If further loaded, the failure and fracture of the membrane and current collector occur. After experiencing these mechanical changes, the positive and negative electrode materials come into direct contact at the fracture points of the membrane and current collector, leading to intense chemical reactions and the occurrence of ISC. This strong electrochemical process releases a large amount of heat. When the internal temperature of the battery rises, several effects are generally observed. Firstly, chemical reactions that occur only at specific temperatures start to take place, such as the decomposition of solid electrolyte interphase (SEI) film and reactions between lithiated carbon and electrolyte solvents, electrolyte decomposition, and

decomposition reactions of the positive electrode. These reactions further release heat and alter the distribution of fluids and solids within the battery. Secondly, the temperature influences the reaction rates and the distribution of chemical species. Some reactions that were originally slow may be accelerated at higher temperatures, leading to further heat generation and forming a vicious cycle. Different temperature distributions correspond to different distributions of chemical species. Thirdly, temperature affects the structural strength and integrity of the battery. Significantly elevated temperatures can cause softening of structural materials, and reactions that generate gas may lead to excessive internal pressure in the battery. This can result in the failure of the weakest points of the battery, leading to the ejection of high-temperature substances and overall structural damage, ultimately causing thermal runaway.

Both the microstructural changes and macroscopic responses of batteries exhibit strong force-electricity-heat correlations. To provide a method that ensures safety and meets cost requirements for studying nail penetration in batteries, Liu et al. developed a multi-field coupled computational approach to simulate the mechanical, electrochemical, and thermal behaviors of wound cores [69]. Jia et al. investigated a decoupling strategy for the coupled mechanical-electrochemical behavior of lithium-ion batteries under dynamic mechanical loads. They explored the mechanical and electrochemical responses of pouch lithium-ion batteries under dynamic loading conditions [70]. Chen et al. reported a combined experimental and computational study on the dynamic response of lithium-ion pouch batteries subjected to high-speed (200–1000 m/s) impact [71]. To gain a fundamental understanding of the failure mechanisms, Yiding et al. proposed a structural-damage-based, coupled mechanical-electrochemical-thermal model. This model was used to investigate the failure behavior of lithium-ion batteries during the mechanical abuse in the hard short-circuit stage at both the real three-dimensional structure and the overall cell level [72]. Liu et al. investigated the evolution of the stress field in a spherical Si/C core-shell structure during the lithium insertion process based on the theory of electrochemical-mechanical coupling [73].

It can be seen that, on one hand, establishing multi-physics coupling models that accurately capture the overall changes of batteries under mechanical abuse is an important trend for future research on the occurrence mechanisms of internal short circuit (ISC) and thermal runaway in batteries. This not only requires us to construct excellent models for individual physical fields but also to choose appropriate strategies for physical field coupling. On the other hand, deformation remains our preferred criterion for failure, which can be defined as the strain value that leads to the failure of separators and the collection electrode reaching a critical spacing.

A 2D multi-physics coupling model based on a strain failure criterion has been developed [74] (Figure 15). In this model, the authors have included several sub-models based on the development process of battery mechanical abuse and the interrelationships among various physical factors. These sub-models include a mechanical model, an internal short circuit (ISC) triggering model, an ISC evolution model, a thermal model, and a thermal runaway model. Although this study has achieved good prediction accuracy for ISC and thermal runaway evolution of batteries under mechanical abuse using a two-dimensional model, it is important to note that batteries are inherently three-dimensional structures. Utilizing a two-dimensional model for research would result in a significant loss of crucial information regarding ISC and thermal runaway that occurs in batteries under mechanical abuse. Therefore, it is necessary to develop a three-dimensional multi-physics coupling model based on strain failure criteria. The bidirectional coupling approach used by Li et al. [72] can more accurately simulate the actual evolution process. By considering the interactions and influences between two or more subsystems, the changes among the different models are bi-directionally connected (Figure 16). This model has been well validated through comparisons with experiments.

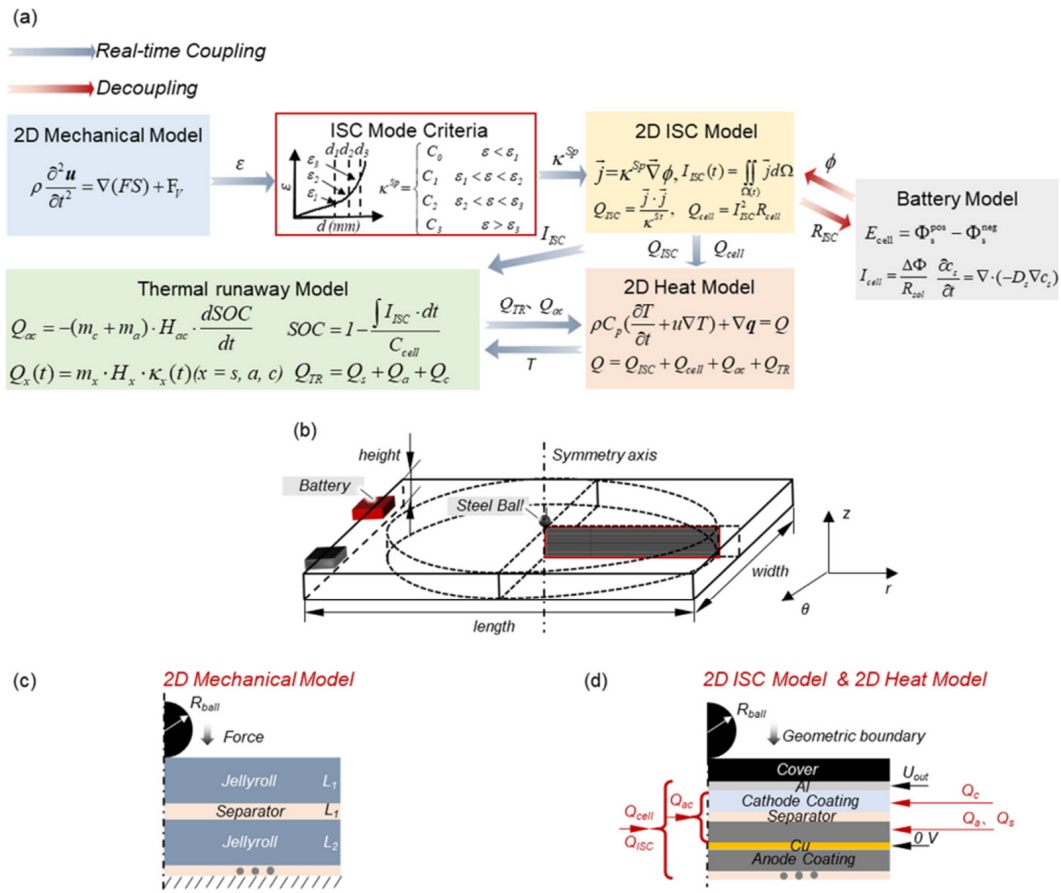


Figure 15. (a) Coupling strategy and schematic algorithms for models, (b) schematics of the geometry of models and boundary conditions for (c) 2D mechanical model and (d) 2D ISC and heat models [74].

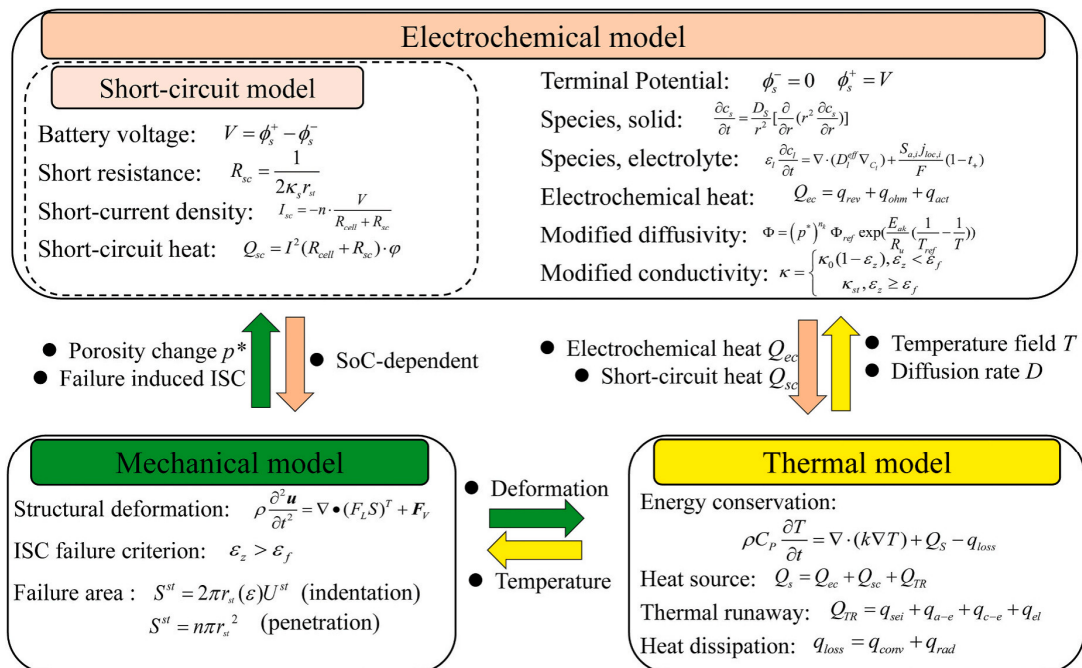


Figure 16. The 3D coupled mechanical–electrochemical–thermal modeling framework for simultaneously simulating the mechanical, electrochemical, and thermal responses of lithium-ion cells under mechanical abuse [75].

Due to the inherent difficulty in in-situ characterization of global information within batteries and the higher cost associated with experimental testing, numerical simulation and modeling of the ISC and thermal runaway evolution of batteries under mechanical abuse through the establishment of a three-dimensional multi-physics coupling model will likely be a promising avenue for future development. Furthermore, as a three-dimensional model entails a larger number of grids and more complex evolution processes, the authors have explicitly represented various components in the model to reduce computational costs without significantly affecting the prediction accuracy. This strategy can be adopted as a method to further deepen the application of numerical computational methods in the future.

3.4. Numerical Optimization for Battery Pack Impact Protection

The previous discussion focused on the numerical simulation research of the mechanical response of individual batteries under mechanical abuse. However, in the development of new energy vehicles, multiple batteries are connected in series/parallel to increase voltage and total capacity, forming a battery pack. If one battery within the pack undergoes thermal runaway, it can easily lead to the propagation of a significant amount of heat and abnormal currents within the battery pack. Therefore, studying the impact resistance of battery packs under mechanical abuse is of great practical significance. With the increasing demand for long-distance driving among consumers, batteries with higher capacity and energy density are being produced and used. The safety risks associated with these battery packs in the event of collisions in traffic accidents are also becoming more severe.

In order to prevent the catastrophic failure of individual batteries and their widespread propagation within a battery pack, current mainstream protection strategies aim to increase the overall strength of the vehicle structure. The goal is to allow as many batteries as possible to absorb the impact energy collectively, thereby ensuring that each individual battery does not bear a load or intrusion beyond its failure threshold. To reduce the economic costs associated with destructive testing using physical prototypes and avoid the safety risks associated with high state-of-charge (SOC), numerical simulation methods have also been successfully applied in this field of research.

Currently, research in academia primarily focuses on the thermal conduction and thermal management issues related to the arrangement of batteries within a battery pack, while there is limited research on the mechanical response and energy conduction mechanisms of battery packs under dynamic impact. Kizilel et al. studied the use of phase change materials (PCM) in a passive cooling system to prevent the propagation of thermal runaway, which can cause catastrophic failure, among adjacent batteries [76]. Kshetrimayum et al. proposed a novel thermal management method for battery modules, involving the integration of phase change materials (PCM) and cooling plates. This method aims to prevent the propagation of heat and thermal runaway within battery modules composed of 18650 battery cells [77]. Chen et al. conducted numerical simulations to evaluate the cooling characteristics of an air-cooled thermal management system for densely packed battery packs under different battery configurations, such as series, offset, and staggered configurations. The aim was to assess the cooling performance of the system for these different battery arrangements [58]. Hu et al. studied the fracture behavior and failure characteristics of packaged batteries. They experimentally investigated the failure behavior of battery packs under quasi-static compression and dynamic collision conditions [78] (Figure 17).

The arrangement of batteries within a battery pack has a significant impact on the propagation and absorption of energy within the pack. Optimizing the energy absorption scheme by altering the layout of batteries in the pack is also a cost-effective optimization option that does not incur additional expenses. In a related study [79], their numerical model was validated through experimental methods. Using the most common arrangement as a baseline, they compared 15 different arrangement schemes with varying types, quantities, and layouts of batteries in terms of energy absorption and battery damage under side pole impact conditions. The study found that, while controlling for the total mass and

volume of the batteries, battery packs with a transverse arrangement were found to be safer compared to those with a longitudinal arrangement. In transverse layouts, the impact energy generated by the side pole can be shared among multiple nearby batteries, whereas in longitudinal layouts, the first battery absorbs the entire impact energy, leading to relatively severe energy dissipation. The study also found that installing thinner batteries in battery packs is safer than using thicker batteries. This is because thinner batteries have lower stiffness, making it easier for them to interact with surrounding batteries through their own deformation and thus distribute energy more uniformly. Essentially, this measure increases the dispersion of the battery pack, reducing concentrated damage. The study suggests that a balance should be struck between the overall stiffness of the battery pack and the local stiffness of individual batteries. However, from a practical standpoint, the study did not simulate specific product batteries but instead used a combination of diverse battery types. This does not fully align with the actual scenario since modern automakers cannot easily adjust the battery supply chain. Therefore, from a controlled variables perspective, limiting the batteries to have the same mechanical response and impact resistance would help investigate the impact of battery cell arrangement on overall impact resistance within the battery pack.

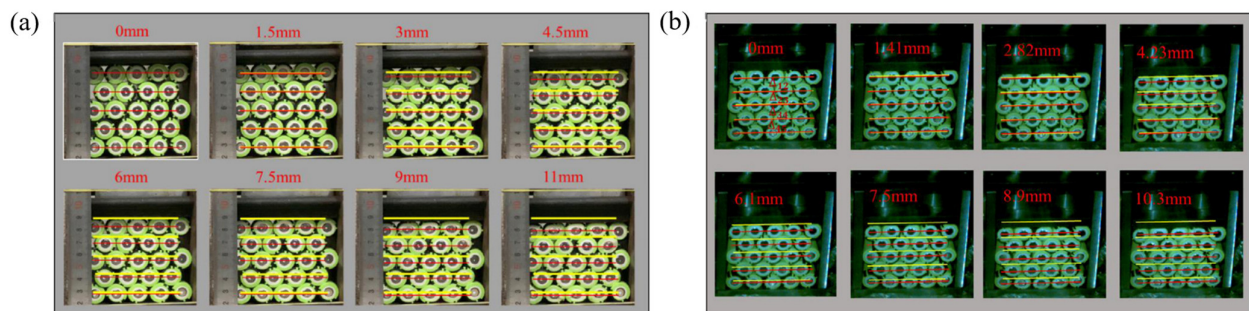


Figure 17. (a) Deformation process of packed batteries under quasi-static; (b) Deformation process of the batteries under dynamic crushing ($M = 9.77$ kg, $V = 11.5$ m/s) [78].

Indeed, further exploration can be conducted on the energy absorption capabilities of battery packs with interleaved battery arrangements. This becomes a potential alternative solution when the energy density reduction resulting from using thinner batteries is deemed unacceptable in commercial competition. The principle behind improving energy dissipation distribution through interleaved layouts involves altering the load-bearing structure of the battery pack to establish additional pathways for load energy transfer. This enables the batteries located away from the impacted end to collectively absorb the impact energy as well.

In the study [80] a homogeneous model was employed to simulate the energy absorption of batteries under three different levels of interleaving. The plastic energy dissipation and deformation of the winding core were used as criteria. It was found that the interleaved layout in Figure 18 not only reduced the energy losses of all winding cores within the battery pack by 7.4% but also reduced the energy losses of the most vulnerable battery winding cores by 2.6–7.4%. The study also found that, under the same level of interleaving, the closer the impact point is to the edge connection of the two batteries, the lower the overall energy dissipation of the battery pack's winding cores. In the case of a 50% overlap ratio, the total energy dissipation of the winding cores was 9.6% lower when the impact point was at the edge of the two batteries compared to when it was at the center of one battery. This indicates that the extent of core damage is highly sensitive to edge effects. This is primarily due to the geometrically vulnerable nature of the shell's boundary region, which is more prone to stress concentration. As a result, the edge junctions between batteries become more efficient pathways for stress propagation. Under this interleaved arrangement, even when choosing the highest degree of interleaving, it only adds an additional 5.1% of excess

space over the conventional layout. Therefore, the impact on the space utilization and energy density of the battery pack is limited.

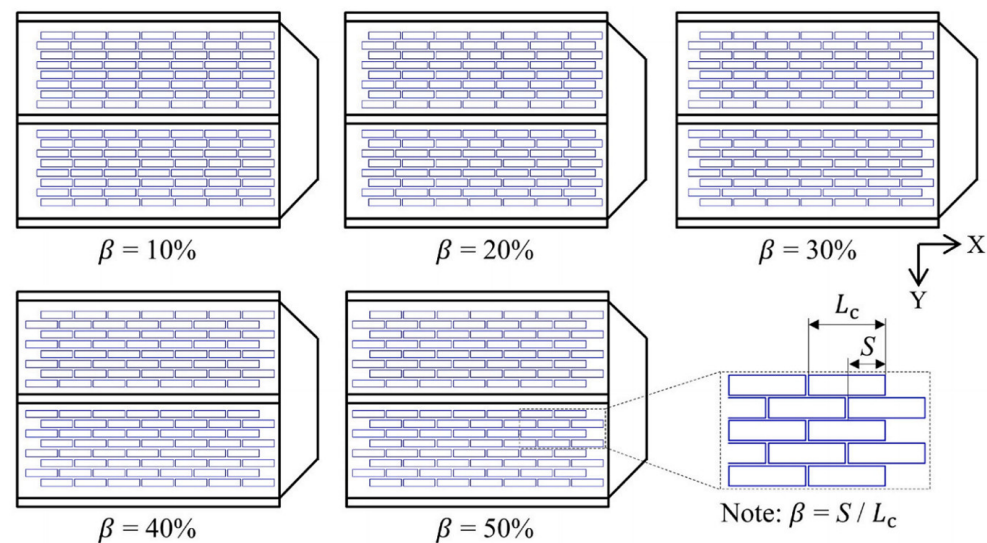


Figure 18. Battery packs with different staggered overlaps [80].

3.5. The Drawbacks of Numerical Simulation Methods Include

3.5.1. Limitations in the Accuracy of Simulation Models

A battery is a microscopically complex multi-field coupled system [81], during the process of modeling, on one hand, it is often necessary to simplify the structural details of the battery according to research needs. While this reduces computational complexity, inappropriate simplifications can lead to inaccuracies in the model. On the other hand, currently, we still lack a complete understanding of the detailed structure and functionality of batteries in practical operation [82], this also poses challenges in establishing accurate models.

3.5.2. Limitations in the Variability of Experimental Data

In order to validate the accuracy of the model, we often rely on a large amount of experimental data for comparison [83]; however, the errors and uncertainties inherent in experimental data can also have a negative impact on model calibration.

3.5.3. Limitation in Complexity of Interfaces

Batteries are composed of stacked layered structures and often contain significant amounts of liquid electrolytes within their solid structures [84], the interaction mechanisms between solid-solid interfaces and solid-liquid interfaces play a crucial role in the operation of batteries [85], The complexity of interface interactions and the lack of comprehensive theoretical studies pose challenges in establishing accurate models and conducting simulations.

3.5.4. Limitations in Computational Complexity and Processing Time

For a complex three-dimensional system like a battery, which is rich in microstructural details, the more accurate and comprehensive the model is, the higher the computational cost will be, posing limitations for related research.

4. Conclusions

A review of safety performance and failure criteria of commercial lithium-ion batteries was conducted, focusing on strain rate and loading direction-dependent mechanical characteristics, SOC-related safety performance, numerical simulation methods and artificial intelligence technologies in battery safety research.

In this article, we first compared the mechanical response of lithium-ion batteries under quasi-static and dynamic loads and identified strain rate dependency as the main reason for

these differences. This indicates that the failure mechanism is different in different loading speed ranges. In the radial compression experiment of the 18650 battery, when the loading speed was low, such as less than 8 m/s, both the inertial effect and stress wave effect were not significant, resulting in overall uniform deformation of the battery with a failure displacement of 6 mm. When the loading speed was medium, typically greater than 8 m/s but less than 40 m/s, the stress wave effect dominated the mechanical response, reducing the failure displacement to 5 mm. When the loading speed was high and larger than 40 m/s, the inertial effect became dominant, causing a rapid failure of the battery due to the instantaneous absorption of a large amount of energy in a small region near the loading end. Furthermore, the researchers also investigated the failure displacement of the 18650 battery under quasi-static loading and determined that the safe compression displacement under axial compression was around 3 mm, while under indentation compression, it was around 6 mm.

The strain rate dependency of the mechanical characteristics of the battery could be explained from the perspective of structure and fluid-structure interaction. The porous honeycomb material constituting the separator itself exhibited a local energy absorption effect, resulting in a pronounced strain rate effect. Additionally, when the liquid electrolyte flows through the porous medium such as the separator, the fluid velocity increases with the increase in load, and the viscous effects inside the pores gradually strengthen, leading to nonlinear increases in viscous resistance and structural damage to the battery. By comparing the mechanical responses of dry batteries and wet batteries under dynamic loads, the researchers found that dry batteries exhibited almost no strain rate dependency under dynamic loads, confirming the fluidic mechanism in the formation of strain rate dependency in lithium-ion batteries.

Batteries in a high state of charge (SOC) are more prone to thermal runaway and unstable voltage fluctuations under mechanical abuse. Mechanical abuse can result in capacity loss and increased internal resistance of the battery. Particularly, when the SOC of a lithium-ion battery reaches 80%, it can also explode under quasi-static loading.

Numerical simulation methods for lithium-ion batteries under mechanical abuse were introduced. The applicability of uniform and detailed models was analyzed and a fault criterion based on displacement for internal short circuits (ISC) and a response evaluation model was proposed. This article outlines coupling strategies for multiphysics modeling. It also discusses the potential application and recent advances of numerical simulation methods in the safety optimization of battery packs. Because the experimental cost is greatly reduced, the application of numerical simulation methods will significantly accelerate the progress of related research.

Through literature research, we can summarize a general approach, such as setting several velocity values from the quasi-static loading speed range to the dynamic loading speed range in experiments with loading speed as the independent variable, to explore the strain rate dependence characteristics of lithium-ion batteries. Additionally, this approach can be extended from studying individual cells to investigating the impact resistance of battery packs, which offers broader application prospects. Researchers can enrich the study by adjusting the shape of the loading head, the loading direction relative to the battery, and other conditions. They can also comprehensively record and analyze the delay of failure occurrence, as well as the evolution of capacity and resistance of the battery during impact. Numerical simulation methods are important for reducing research costs and enriching research content. Researchers should attempt to establish numerical models and refine them with data obtained from experiments. This will enable the use of more accurate models to study a greater variety of complex operating conditions, leading to deeper exploration of the research subject.

Finally, artificial intelligence technology is expected to be widely applied in various industries. However, there is still a lack of literature reporting the use of relevant methods for impact protection and safety research of lithium-ion batteries. This is because the complex material and structural characteristics of lithium-ion batteries, as well as the

presence of multiple physical fields, make it difficult to accurately characterize them. As a result, the advantages of artificial intelligence methods cannot be fully highlighted. Another reason is that artificial intelligence methods require a large amount of data to train the algorithms, which is currently lacking in the early stages of research in this field. However, there is no doubt that artificial intelligence methods have demonstrated their unique advantages and strong development trends. This will undoubtedly be a key direction for future researchers in the field of battery safety to explore.

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