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A Review on the Development and Research Methods of LIB and SEI

Xiaotian Zhu

China University of Mining and Technology, Xvzhou, China
19852490816@163.com

Abstract. In the context of global energy transition, lithium-ion batteries, as the core of the new energy industry, have always attracted much attention due to their performance and safety issues. The thermoelectrochemical coupling effect generated during the operation of lithium-ion batteries, as well as the characteristics of the solid electrolyte interface (SEI) film, have a direct and crucial impact on the lifespan, performance, and safety of the batteries. The world is currently promoting energy transition, and lithium-ion batteries are the core component in the new energy field. Everyone is very concerned about whether their performance is good and whether they are safe to use. In addition, during battery operation, there is a thermoelectrochemical interaction, and a substance called SEI film is involved. These two factors have particularly direct and crucial influences on how long the battery can be used, its performance, and its safety level. And numerical simulation methods not only require fewer resources but also have a shorter experimental cycle. Nowadays, they have become an important means for studying the thermal behavior during the discharge process of lithium-ion batteries.

Keywords: component, LIB, SEI, thermal behavior, thermal management systems

1. Introduction

In the context of global energy transition, lithium-ion batteries (LIBs) can be regarded as the most crucialfundamental component in the rapidly developing energy sector. Moreover, when LIBs are in operation,a phenomenon called "thermoelectrochemical coupling effect" occurs. This effect significantly impactsthe performance and safety of the battery - this is one of the fundamental issues that need to be focusedon in subsequent studies such as SPM model optimization and BTMS design. Moreover, since the SolidElectrolyte Interphase (SEI) concept emerged in 1989, research has evolved from observational inquiryto intricate mechanistic exploration. Presently, it is widely recognized that SEI film formationencompasses two processes: initially, battery negative electrode polarization instigates reductivedecomposition of electrolyte components; subsequently, nascent products precipitate on the electrode'ssurface, engendering the SEI film [1].

In the research on the formation mechanism of the SEI film, the controversies mainly focus on the reduction conversion process of electrolyte solvent molecules. There are three possibilities for this process: first, individual lithium ions are directly intercalated into the graphite layers of the negative electrode during the reduction conversion, completing the intercalation [2]. The second one is based on the assumption by Aurbach et al. that the reduction conversion of solvent molecules is a one-electron conversion, generating an intermediate product—a radical anion. This anion further decomposes and combines with lithium ions to form precipitated substances, which become components of the SEI film [3]. According to the assumptions by Dey, Besenhard, Chung et al., during the co-intercalation of lithium ions and solvent molecules, the solvent molecules undergo a two-electron reduction conversion. There is a rather weak "attraction" (that is, van der Waals force) between lithium ions and solvent molecules. They first come together through this force, and then together squeeze into the gaps between graphite layers. Thus, an intermediate substance is formed, called a ternary graphite intercalation compound. This intermediate product is then reduced to form the SEI film. The third possibility is that electrons from the negative electrode are directly transferred to the anionic salt, and inorganic salt precipitates are directly formed with lithium ions [4-6].

The SEI film, a nanoscale barrier safeguarding lithium-ion batteries' negative electrode and electrolyte interface, considerably influences battery longevity, efficiency, and safety, thereby emphasizing its significance for performance augmentation. SEI film quantity embodies lithium depletion within the battery, dictating its comprehensive capacity. Suboptimal electron insulation properties of the SEI film during cycling permits electron-electrolyte contact, provoking reduction conversions that exhaust lithium, stimulating SEI film formation, and diminishing battery lifespan [7]. Two noteworthy phenomena—peeling and thickening—can unfold in the SEI film during cycling. When peeling materializes, SEI film particles infiltrate the electrolyte and succumb to electrophoresis under voltage influence, heightening particle deposition on electrode surfaces throughout high-rate discharge. Simultaneously, SEI film thickening manifests during high-rate cycling, exacerbating electrode impedance, impeding lithium efflux, and constraining rate performance [8,9]. As lithium-ion batteries undergo rapid charging, lithium-ion transit across the SEI film lagging behind deposition on the negative electrode potentially cultivates continuous lithium dendrite formation over successive cycling cycles, elevating the risk of short circuits and consequent combustion or explosions. Moreover, an incomplete or deteriorated SEI film provokes lithium-electrolyte-binder conversions upon intercalation into the negative electrode, discharging heat commensurate with intercalated lithium—a critical arbiter of battery safety [10].

Numerical simulation methods, with advantages such as low resource consumption, short experimental cycles, precise control of variables, and the ability to test extreme operating conditions, have been widely applied to explore the thermal behavior during the discharge process of lithium-ion batteries.

Current simulation studies of lithium-ion batteries predominantly center on thermal behavior during charging and discharging, SEI film dynamics, and cathode material chemical characteristics. Increasing attention is being afforded to the thermal resilience of the SEI film, yet a void persists regarding comprehensive appraisals of its robustness. Alongside thermal resilience, it is critical to assess the interplay between SEI film structure and performance, as it substantially shapes strategies for bolstering battery safety and longevity.

Therefore, a comprehensive review and analysis of studies on the thermal behavior during charging/discharging and the SEI film are vital for the future development of lithium batteries [11].

This paper selects lithium-ion batteries as the research object and summarizes the research results on the thermal behavior during battery charging/discharging and the thermal resilience of the SEI film in recent years from two directions. Different from other review articles, this paper focuses on battery model establishment and numerical simulation in the current research field, discusses the reference value and room for progress in model establishment and numerical simulation, and proposes that factors such as thermal condition field distribution caused by the thermal behavior during charging/discharging are of research value concerning the interdependencies between structural attributes and functional performance of the SEI film. It also puts forward future research directions for the SEI film, with a focus on structural design and further robustness studies. This paper is expected to be of great value for the development of cathode materials and structures with higher thermal resilience and excellent electrochemical performance, as well as thermal management systems. It will contribute to the progress of lithium battery development, accelerate their commercialization, promote the transition from traditional fossil energy to new energy, and drive global sustainable development.

2. Review of achievements analysis on past thermal behaviors of LIBs

2.1. Review of research on thermal behavior of battery charging and discharging (mathematical model establishment)

Lithium-ion batteries (LIBs) generate a substantial thermal output throughout charging and discharging processes, leading to changes in the overall thermal condition. This, in turn, affects the capacity and performance of the batteries. In some extreme cases, it may even trigger thermal escalation, resulting in major safety accidents. To meet the specific requirements of lithium-ion batteries, especially in terms of thermal safety, researchers have invested significant efforts over the past few decades in studying the thermal disposition of lithium-ion batteries throughout energizing and de-energizing phases and exploring the influencing factors of such thermal behavior.

Previous in-depth studies have discussed the impact of thermal condition distribution on LIBs during operation. Reference [12] indicates that LIBs perform optimally within the thermal condition range of 293.15 313.15 K represents the ideal thermal window for battery operation, as thermal conditions straying beyond this range adversely impact performance. Exceeding 333.15 K, charging and discharging efficacy markedly declines, potentially triggering thermal escalation events with perilous consequences [13].

If further study the temperature field distribution inside the battery pack, we will find that it has a particularly significant impact on the performance of LIB. Here is a crucial point: the temperature difference between batteries must be controlled within 5K. Because if the temperature difference between the batteries is too large, it will seriously slow down the overall performance of the battery pack - this is actually related to the previously mentioned thermoelectrochemical coupling effect, BTMS design, etc., all of which are centered around "improving the performance and safety of LIB" [14].

To keep the battery operating within its optimal temperature range and ensure a uniform temperature distribution within the battery pack, it is particularly crucial to equip it with an efficient battery thermal management system (BTMS). This system not only enables the battery to perform at its best but also extends its lifespan and reduces the risk of thermal runaway. This is particularly important for ensuring the overall reliability of the battery, just as optimizing the SEI layer, improving the silicon-based electrode, and so on, are all key steps in enhancing the performance and safety of LIBs. It also perfectly aligns with the requirement we just discussed of "controlling the temperature difference of the battery within 5K and avoiding slowing down the performance of the battery pack" [15].

The current mainstream methods for battery thermal management systems (BTMS) mainly include air cooling, liquid cooling, phase change material (PCM) cooling, and heat pipe (HP) cooling [16]. These approaches can provide certain assistance and offer some reference ideas for future battery design and the development of new BTMS methods - after all, as we previously mentioned, BTMS is particularly crucial for controlling battery temperature, ensuring performance, and maintaining safety. In this section, we also reviewed the "electrochemical-thermal coupling model" used in recent research, discussed the influence of lithium-ion battery thermal behavior, and how to regulate it. These efforts aim to provide valuable guidance for future research on lithium-ion battery thermal behavior and the establishment of related models. After all, in this field, there is no yet a complete data system, and there are still many areas that need to be improved.

2.2. Review of the establishment of traditional electrochemical-thermal coupling models

Physics-driven electrochemical models for battery simulation seek to decode delineating complex battery functioning entails unraveling electrochemical mechanisms and transport phenomena occurring within batteries throughout cycling sequences, promoting detailed performance insights. Electrochemical-thermal coupled battery models present a potent, resourceful blueprint for LIB exploration at the cellular level, comprising current collectors, cathodes, separators, and anodes. These models furnish dependable numerical outcomes, circumventing intricate experimental analyses for battery characterization [17].

As foundational elements of other battery frameworks, these models proficiently capture internal disparities of individual battery cells [18].

The realm of physics-driven electrochemical models for battery simulation encompasses a gamut of complexity, epitomized by the Single Particle Model (SPM), Newman Pseudo-2D (P2D) framework, and Doyle-Fuller-Newman (DFN) methodology. These methodologies furnish nuanced insights into battery dynamics, allowing for multifaceted examination of performance attributes. To simplify the battery representation, the SPM describes each electrode through a singular emblematic particle. This paradigm fixates on lithium-ion conveyance within solid electrode particles and conversion kinetics at the electrode/electrolyte junction. It eschews electrolyte transport and postulates homogeneous lithium-ion dispersion within the electrolyte [19].

The commonly used single-particle model (SPM) in the industry, even after optimization through equivalent circuit models (ECMs), usually does not assess the battery's thermal output – because the influence of electrolyte kinetics on the thermal output has not been fully considered (which may cause a significant decline in battery performance). The effects of open-circuit voltage (OCV), internal resistance, and temperature on the discharge capacity in the SPM need to be further studied. They can interfere with parameters such as diffusion coefficients and may affect the model's accuracy. The correction method is not complicated: extract the correlations between OCV, internal resistance, and temperature from experimental data, and integrate them into a regression function [20,21]. This approach can make up for the shortcomings of the SPM, provide a reference for subsequent modeling, and is consistent with the idea of BTMS controlling temperature to optimize battery performance.

The Doyle-Fuller-Newman (DFN) model exemplifies a quintessential electrochemical model [22]. Extending the P2D framework, DFN harnesses the Nernst-Planck equation to encapsulate intricate lithium-ion transport within electrolytes, incorporating concentration-dependent diffusion and migration facets. While the model furnishes an exhaustive portrayal of battery electrochemistry, it concurrently bears computational intricacy and notable resource intensity [22].

To deconstruct electrochemical models, we resort to block diagrams, as exemplified in Figure 1 [22]. Parenthetically, the reference denotes model components (e.g., PDE, ODE, explicit expressions) and ensuing spatial discretization (e.g., DAE or ODE). Block color signifies model intricacy: red embodies differential-algebraic expressions (DAE, elevated intricacy), yellow embodies standard differential equations (ODE, medium intricacy), and green denotes explicit notations (low intricacy). Readers can peruse color references in the aforementioned legend at [23] in this article.)

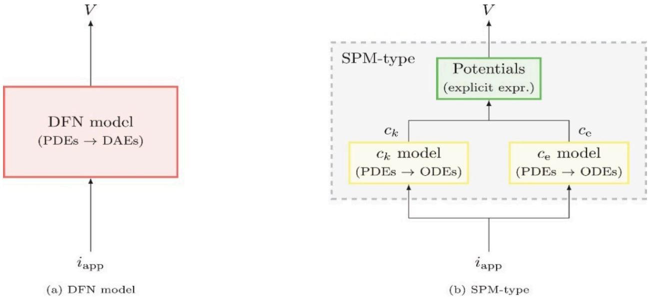

Figure 1. (a)DFN model (b)SPM-type [22]

The Newman P2D model, a simplified DFN derivative, enjoys widespread employment in physics-grounded electrochemical-thermal simulations. P2D captures intricate electrochemical processes during battery cycling whilst exhibiting moderate computational resource demands. Nonetheless, its premise of dense, homogeneous, monodisperse, and impeccably spherical active material particles risks misrepresenting electrode characteristics [24]. Storage, 104(PB), 114755-114755. Therefore, the Newman P2D model achieves a relatively high level of accuracy without excessive intricacy in its construction. Due to the intricacy of the P2D model, independent compilation and solution can be challenging. Hence, commercial CFD software packages integrated with the P2D model, such as COMSOL Multiphysics, are widely used to build physics-based electrochemical battery models. By referring to numerous references [25-32], it is found that most couplings occur between 1D (P2D) electrochemical models and 3D thermal models. Leveraging the 1D model-derived heat generation rate as a thermal source, the 3D model meticulously maps the battery's internal thermal condition landscape. Consequently, mean thermal condition yielded by the 3D framework impinges upon the 1D electrochemical model, constructing a feedback circuit. Such thermo-electrochemical parameter sensitivities to thermal condition modulations underlie this interplay, reciprocally influenced by thermal condition elevations [27,33,34,35].

Despite its potential, scant investigations employ the P2D model for FLUENT-based thermal scrutiny of lithium batteries in FLUENT [35-37]. While COMSOL excels at navigating multi-physics predicaments inherent to battery electrochemical models, FLUENT outshines COMSOL for resolving fluid dynamics and thermal transfer frameworks. Therefore, the application of FLUENT can be of great help in analyzing the thermal condition field distribution of electrochemical models or in establishing thermal management systems. Figure 2 shows a contour map of the spatial pressure distribution of water flowing over a 2D flat plate, constructed using ANSYS FLUENT. Additionally, FLUENT can be used to display indicators such as thermal condition and flow velocity.

In summary, the Single Particle Model (SPM) simplifies the process by neglecting factors such as electrolyte concentration gradients, using a "single particle" to represent electrode particles, and reducing partial differential equations to ordinary differential equations. It is only accurate under low-rate (≤1C) and steady-state operating conditions, and can complete calculations in milliseconds to adapt to the real-time control of the Battery Management System (BMS). Thus, it is an efficient but highly simplified real-time estimation tool.

The Doyle-Fuller-Newman Model (DFN) fully accounts for all core physicochemical processes, including the porous structure of electrodes and electrolyte transport, enabling the study of complete mechanistic outcomes. It can accurately simulate internal changes under complex operating conditions such as high rates. Although more precise, it requires high-performance computing equipment and can take hours or even days to complete calculations.

The Pseudo-Two-Dimensional Model (P2D) retains the two-dimensional coupling of "particle radial diffusion + electrode axial transport" and only ignores some microscale inhomogeneities, ensuring both the relative accuracy of results and reduced computational complexity.

Therefore, the three models have distinct focuses in their core application scenarios: SPM is suitable for real-time State of Charge (SOC)/State of Health (SOH) estimation in electric vehicle BMS; DFN is used for mechanistic research such as battery electrode material design; and P2D plays a role in engineering scenarios such as the optimization of battery pack charging and discharging strategies.

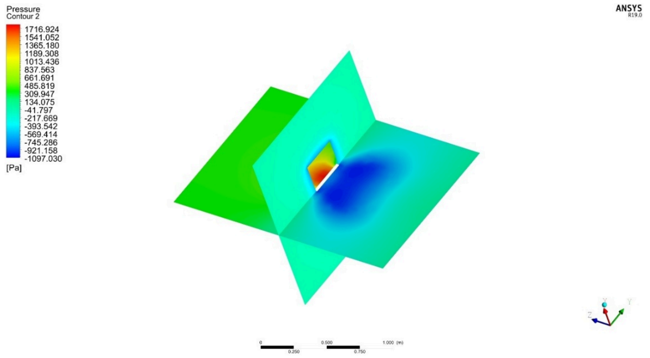

Figure 2. An ANSYS FLUENT 2D flat plate

3. Review on the research of cathode SEI films (numerical simulation)

3.1. The formation mechanism of SEI and its influence mechanism on battery thermal behavior

The Solid Electrolyte Interphase (SEI) film in Lithium-ion Batteries (LIBs) emerges as a nanoscale membrane, engendered via electrolyte decomposition and conversion. During nascent LIB cycling episodes, SEI coalesces at the electrode material-electrolyte solid-liquid nexus. Regulating lithium ion conductance while impeding electron-electrode contact, SEI stands as a lynchpin of battery long-term robustness. SEI formation progresses through three cardinal stages: incipient development, expansion, and reconfiguration (Fig. 3d) [38].

Upon nascent lithium metal anode-electrolyte interaction, reduction byproducts on the electrode surface trigger conversions with electrolyte solvents and salts, producing an amalgam of organic and inorganic composites. Accumulating on the electrode surface, these compounds forge an incipient SEI film, passivating the anode surface. Notwithstanding, the initial SEI's suboptimal electronic insulation facilitates persistent reduction conversions, propagating SEI growth via film thickness augmentation. Throughout electrochemical cycling, recurrent anode volume fluctuation (expansion-contraction) underpins SEI dynamism and evolution [39].

If the SEI lacks sufficient mechanical robustness, it may crack or reconstruct. In this process, organic compounds can be oxidized into carbonates, polymers, and oxides, and inorganic salts can form stable precipitates with lithium ions. Achieving an SEI with mechanical robustness and chemical passivation is essential for ensuring the long-term performance of the battery.

Under normal operating conditions (typically < 80°C), the SEI film can stably prevent the direct reaction between the electrolyte and the electrode. However, when the temperature rises (e.g., due to local heating caused by overcharging or short-circuiting), if the SEI film has poor thermal stability, it will decompose first at a relatively low temperature (approximately 90-120°C), releasing gases such as CO_2 and CH_4 and exposing fresh active surfaces of the electrode. These fresh surfaces then undergo violent exothermic reactions with the electrolyte, rapidly increasing the internal temperature of the battery, directly triggering more dangerous subsequent thermal behaviors and lowering the threshold temperature for battery thermal runaway.

The thermal decomposition of the SEI film is a key exothermic link in the early thermal behavior of the battery: An SEI film with poor thermal stability decomposes at a high rate and releases heat in a concentrated manner, leading to a sudden rise in the battery's internal temperature. This accelerates chain reactions such as electrolyte evaporation and separator shrinkage/fusion, quickly escalating the thermal behavior from "mild heat release" to "violent deflagration". In contrast, an SEI film with good thermal stability decomposes gently and releases heat in a dispersed way, which can slow down the rate of temperature rise, prevent the thermal behavior from getting out of control in a short time, and even allow heat to be dissipated through the thermal management system to avoid thermal runaway.

After the SEI film fails due to thermal decomposition, it not only loses its interface protection function, but also its decomposition products may undergo secondary exothermic reactions with other substances in the battery. These reactions superimpose the initial exothermic effect, transforming the battery's thermal behavior from a "single interface reaction" to a "multi-link coupled exothermic reaction", and ultimately leading to the spread of thermal runaway.

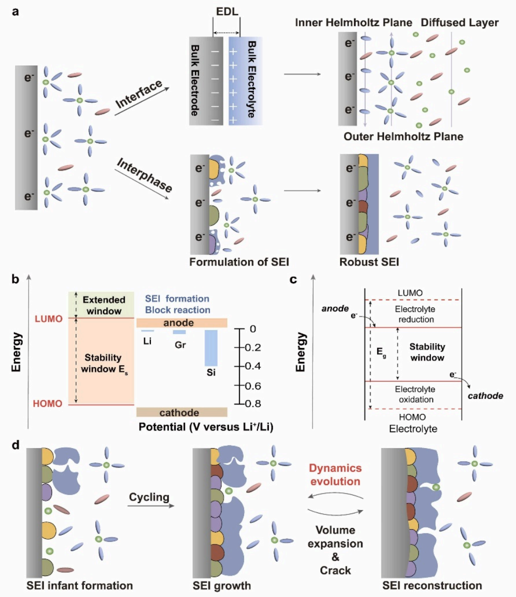

Figure 3. The conceptual schematic (Fig. X) dissects "interface" and "interface" paradigms while expounding SEI formation processes: (a) distinguishing interfaces and interfaces, SEI formation mechanisms and progression; (b) HOMO/LUMO energy echelons and operational voltages of co-anodes (Li, Gr, Si); (c) Accurate symbols for electrolyte robustness cathodic and anodic potential boundaries. Reprinted with authorization [40].All rights reserved 2018, The Royal Society of Chemistry. (d) SEI formation process.

3.2. Investigation on the thermal resilience of SEI films

SEI film ramifications on battery safety stir significant apprehension. The SEI film exhibits marked thermal sensitivity, particularly under thermal condition extremes, with potential consequences for battery performance under such conditions. Elevated thermal conditions incite side conversions that escalate SEI thickness, compromising battery capacity [41].

The SEI film can maximize the inhibition of lithium dendrite formation under overcharge conditions. Therefore, it is crucial to minimize the heat escalation of the battery caused by the decomposition of SEI components at high thermal conditions. An ideal SEI film should have properties such as high resistance, high lithium-ion selectivity, high mechanical stress to limit the enhancement of lithium dendrites, the ability to adapt to the expansion and contraction of anode materials during battery cycling, insolubility in electrolytes, and stable operation over a wide thermal condition and voltage range. However, the actual SEI does not meet these requirements, and the regulation of SEI remains a major direction in the study of lithium-ion batteries in the future.

Regarding the thermal decomposition process of the SEI film, numerous research so far. In the early stage, Zhao et al. [42] used TG-MS to study the changes and gas production of the SEI on the graphite anode of LIB during the heating process, and Yamaki et al. [43] used DSC to study the thermal resilience of the SEI with electrolyte in LIB. Recently, Huang et al. [44] investigated the variation of the morphology, mechanical properties, and chemical construction of the SEI with thermal condition using techniques such as AFM and XPS. They found that as the thermal condition increases, the Young's modulus and particle size of the SEI gradually increase, indicating the decomposition of unstable organic substances therein, which provides a deeper understanding of the thermal changes of the SEI. Ouyang et al. [45] used synchrotron radiation XRD andand in-situ mass spectrometry techniques unveiled the thermal degradation dynamics of lithiated graphite anodes, encompassing SEI decomposition, lithium deposition, and gaseous byproduct evolution. Notably, combustible gases like H_2 were identified and quantified, emphasizing the SEI's pivotal role in anode thermal resilience. These insights underscore latent perils stemming from combustible effluent release and leached lithium, accentuating the need for enhanced thermal management strategies in LIBs. From these studies, it is known that some unstable organic components in the SEI film will gradually decompose and release gases at high thermal conditions, but their specific composition and structural changes still need further research.

Wu revealed the inherent thermal resilience of the SEI film from aspects such as decomposition pathways, phase transitions, microstructure evolution, and gas release. The SEI membrane itself is "sensitive to heat" and can decompose into carbon dioxide even at room temperature. Once the temperature rises, the organic substances and LixPOyFz within the membrane will decompose, releasing flammable gases and generating heat. This can easily precipitate a perilous "thermal escalation" scenario within batteries where the heat is uncontrollable [46].

The research conducted by the Teng team indicates that when various substances in the battery undergo exothermic reactions, the reaction between the positive electrode and the electrolyte is particularly crucial. Notwithstanding the recognized significance of heat generated through negative electrode-electrolyte interactions, a nuanced perspective must account for the negative electrode's thermal conductivity, given its potential to incite battery overheating. Notably, thermal changes intrinsically influence gas production tendencies irrespective of electrode polarity, accentuating the need for comprehensive thermal regulation to preserve optimal battery performance [47].

Some researchers also conducted experiments using different materials, aiming to find suitable materials to enhance the thermal resistance of electrode materials. For instance, the Wang team added four specific additives - vinyl carbonate (VC), 1,3-propionoic acid ester (PS), MMDS, and vinyl diacetate (DTD) - to create a sulfur-rich composite electrolyte. The experimental results showed that MMDS and DTD were quite effective: they could lower the temperature at which the electrolyte undergoes thermal decomposition (making the electrolyte less prone to decomposition due to high temperature), enhance the battery's rate performance, and improve the battery's stability in high-temperature environments. Later, through SEM (scanning electron microscope) and FTIR (infrared spectroscopy) analysis, it was further confirmed that these four additives – VC, MMDS, DTD, and PS - had positive effects: they could promote the reduction reaction on the surface of the graphite negative electrod, forming a stable SEI film, and also enhance the thermal resistance of this film [48].

Yu Zheng et al. developed a porous composite film made of polyetherketone nitrile (PENK) and polyvinylidene fluoride (PVDF). The research results showed that the addition of LLZTO can significantly improve the wettability, thermal resilience, and cycle performance of the electrolyte, and the optimized PENK/PVDF composite film exhibits excellent thermal resilience [49].

The aforementioned investigations encapsulate prevailing research trajectories and methodologies centered on the thermal robustness and thermal attributes of the SEI film. These inquiries predominantly concentrate on electrolyte and electrode material advancements to optimize thermal stability and performance, the synthesis of SEI films with stable properties, and the improvement of the thermal resilience of batteries. In addition, it is found that, for example, the composition and structural changes of the unstable structures generated in the SEI film are still not very clear and require further research. When designing suitable electrode materials and electrolytes, numerical simulation calculations and modeling can also be used to design theoretical models to simulate the working conditions of the battery.

Of course, improving the thermal stability of the SEI is not only greatly helped by the selection of electrode and electrolyte materials; we also need to find more suitable thermal management systems to enhance thermal stability. Currently, the systems for controlling the thermal stability of the SEI include air cooling, liquid cooling, phase change material cooling, and heat pump technology.

3.3. Structure-performance relationship of SEI films

Recent scholarly endeavors have delved into the intricate interplay of electrochemical and mechanical attributes in the Si-C system through an amalgamation of experimental and modeling techniques, researchers investigate the composite battery system. While empirical studies have chronicled diverse interface debilitation mechanisms [50], prevailing scholarship predominantly centers on particle-scale active materials [51-55], adopts oversimplified macroscopic postulations [56], or spotlights exclusively electrochemical dimensions. This landscape reveals a deficiency in harmonized methodologies addressing volumetric expansion, plastic flow, and interfacial degradation under finite strains.

If there is inefficiency with the battery interface, it is very likely that the SEI layer is causing the issue. The research team conducted a detailed analysis of the silicon-carbon electrode and found that if the amount of silicon exceeds the limit, the SEI layer will be under excessive pressure and may "fail". As for whether the SEI layer will completely stop functioning, it mainly depends on two aspects - whether its own strength is sufficient and its stability is good, and whether it can firmly "attach" to the electrode. These research conclusions can provide assistance for the improvement of the material and performance of the silicon-based electrode, thereby making the battery more reliable. In addition, the improvement directions for the structural properties of SEI can be divided into the following points: (1) Exceptional chemical/electrochemical steadfastness: Chemical constancy precludes unwanted conversions, while electrochemical robustness ensures electronic isolation—both pivotal for efficient battery operation. (2) Enduring mechanical strength and pliancy: Volume shifts throughout cycling can incite SEI fractures, catalyzing side conversions that substantially erode performance. (3) Exemplary ion transport: Uniform lithium mobility within the SEI is vital for reliable deposition and superior rate capability.

4. Discussion and conclusion

Based on the results and discussions presented above, the conclusions are obtained as below:

1.Thermal behavior during cycling cycles and model research: The heat generated during LIB cycling cycles affects battery capacity and performance, and may even trigger thermal escalation. The optimal operating thermal condition range is between 293.15 K and 313.15 K, and the thermal condition difference within battery packs must be controlled below 5 K. An efficient battery thermal management system (BTMS) is crucial for maintaining battery performance, extending lifespan, and preventing thermal escalation, with mainstream technologies including air cooling and liquid cooling. Physics-based electrochemical models (e.g., SPM, DFN model, Newman P2D model) play an important role in battery simulation, among which the coupling of 1D (P2D) electrochemical models with 3D thermal models is widely applied. Additionally, FLUENT shows potential in analyzing thermal condition field distribution and thermal management systems.

2.Research related to the SEI film: When batteries are recycled, several factors can affect the SEI membrane. For instance, if charging and discharging occur too rapidly (high-speed cycling), the battery's storage capacity will decrease more rapidly; if the discharge speed is too intense, not only will the amount of lithium decrease due to the formation of the SEI membrane, but the SEI membrane will also become less sturdy, and even the active materials in the electrode will be damaged; if the electricity is discharged too thoroughly (over-discharging), it will also cause problems such as the reformation of this structural damage of the SEI membrane. Additionally, during the battery recycling process, heat is generated, and the temperature distribution formed by this heat may also have an impact on the structural stress of the SEI membrane.

3.Future research directions: When conducting research on SEI membranes, the key points to focus on are: first, the structure of the membrane must be designed properly; second, the stability of the membrane needs to be studied in greater detail. In addition, there are two other crucial aspects: on one hand, it is necessary to understand the thermal characteristics of the battery during repeated charging and discharging, and the relationship between the internal structural stress field of the SEI membrane; on the other hand, the relevant models and simulation methods need to be optimized. By completing these tasks, it will be possible to provide support for the development of better cathode materials, battery structures, and thermal management systems, thereby promoting the development of lithium-ion battery (LIB) technology and commercialization, and contributing to global energy transition and sustainable development.

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