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Interface Chemistry: A Review of Strategies for Lithium Battery Interface Control and Dendrite Suppression

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ABSTRACT
The performance and lifespan of lithium batteries depend on the stability of the electrode-electrolyte interface. This paper focuses on analyzing the mechanism by which interfacial chemistry suppresses dendrite growth through interface regulation. Uneven ion distribution on the electrode surface and defects in the SEI film can trigger lithium dendrite growth. Constructing an artificial SEI film, optimizing the electrolyte, and developing three-dimensional current collectors can promote uniform lithium deposition. High-concentration electrolytes can modulate solvation structures, while surface coating treatments and interface stress management strategies also effectively suppress dendrite formation. Current challenges include unclear interfacial mechanisms and imperfect manufacturing processes. Future efforts should advance multi-scale characterization, leverage machine learning for design optimization, and achieve synergistic improvements between interfaces and bulk materials. These findings provide critical support for designing high-energy-density, safe lithium batteries.

KEYWORDS
Interface chemistry; Lithium batteries; Interface regulation; Dendrite suppression; Strategy

1 Research background

1.1 Research significance of lithium batteries and electrode reactions

In the field of modern energy storage, lithium batteries occupy a central position, with their performance and safety being of paramount importance. Lithium metal anodes are regarded as the ideal choice for breaking through the energy density bottleneck [1], owing to two key characteristics: first, a high specific capacity of 3860 mAh/g, and second, a potential of -3.04 V (compared to the standard hydrogen electrode, SHE). These properties correspond to high specific capacity and low potential, respectively. However, interface instability can cause uneven Li^+ deposition and subsequent dendrite growth, potentially triggering short circuits and thermal runaway [2]. Research indicates that electrochemical polarization causes Li+ to deposit preferentially at protrusions, and defects in the SEI film exacerbate this uneven transport [3]. When current density exceeds critical values, localized concentration gradients form, accelerating dendrite growth [4]. In liquid electrolytes, side reactions generate brittle organic solid electrolyte interphase (SEI) films, continuously depleting active lithium [1]. While solid electrolytes mechanically impede dendrite growth, solid-solid interfaces exhibit low ionic conductivity, potentially allowing dendrites to penetrate along grain boundaries [5]. Addressing these challenges, interface chemical regulation offers novel solutions. For instance, constructing engineered SEI films or modifying current collector surfaces can enhance Li^+ nucleation behavior [6-7], thereby facilitating a transition from dendrite growth to uniform deposition.

1.2 Analysis of dendrite growth issues

Multiscale dynamic instability at the electrode-electrolyte interface triggers lithium dendrite growth. At the microscopic level, Li^+ nucleation on the electrode surface is not uniformly distributed, influenced by local current density and the heterogeneity of the SEI film. Yang Jiayue's team observed that surface defects amplify electric fields, leading to preferential nucleation of dendrites [2]. Research by Wen Xinyi's group revealed that dendrite morphology is determined by the ratio of Li^+ deposition rate to diffusion rate: a higher ratio yields needle-like dendrites, while a lower ratio produces moss-like structures [3]. At the mesoscopic level, modulating SEI film properties drives dendrite evolution. Shi Min's team noted that SEI films formed from liquid electrolytes are prone to rupture, triggering side reactions [1]. Wang Zixuan's team discovered that while solid electrolytes mechanically block dendrites, stress concentration at their interfaces may promote dendrite growth along grain boundaries [5]. At the macroscopic level, three failure scenarios exist: short circuits caused by separator punctures, capacity degradation due to dead lithium accumulation, and increased interfacial impedance. Hou Pengyang's team simulated that dendrite growth rates decrease with rising temperatures and exhibit a nonlinear relationship with stress [4].

1.3 Limitations of traditional methods for inhibiting dendrite growth

Traditional methods for suppressing lithium dendrites have significant limitations. The SEI film formed in liquid electrolytes exhibits mechanical inhomogeneity, making it prone to rupture and triggering side reactions [1]. While the additive VC can stabilize the SEI, excessive use leads to decreased ionic conductivity [3]. In physical suppression methods, excessive external pressure causes dendrites to spread laterally, a scenario where ceramic separators struggle to accommodate volume changes [8]. Within all-solid-state batteries, stresses at the solid-crystal interface further facilitate dendrite penetration [5]. Three-dimensional current collectors can reduce current density, but their structures are relatively complex and prone to collapse[7]. Additionally, Li^+ coatings exhibit poor long-term stability [9]. These approaches lack dynamic regulation capabilities, making it difficult to meet the demands of high energy density.

2 Research content

2.1 Homogeneous lithium deposition

For suppressing dendrite growth, homogenizing lithium deposition is a critical strategy. Through phase-field simulations, Yang Jiayue's team discovered that localized electric field enhancement occurs at micro-asperities on the electrode surface, causing Li^+ to deposit preferentially at these sites and form dendrite nuclei [2]. In response, researchers developed multiple interfacial engineering strategies: Regarding current collector modification, three-dimensional porous structures effectively increase specific surface area, thereby significantly reducing local current density. Lin Yu's team confirmed that applying lithium-affinity coatings to copper current collectors reduces lithium nucleation overpotential by approximately 60%, promoting uniform nucleation [7]. Jin Caiyun's team developed a phosphorazide-based artificial interfacial layer (SHP) that utilizes nanoporous confinement effects for selective Li^+ transport. Its distorted molecular chain structure homogenizes ion flow distribution [9].

Optimizing electrolyte composition critically impacts deposition uniformity. Shi Min's team demonstrated that elevated electrolyte concentrations alter Li^+ solvation structures, causing free solvent molecules to disrupt the SEI film and form stable interfacial layers containing inorganic components [1]. Wang Ce's team discovered that sulfonic acid-based covalent organic framework material (COF-1) can increase the Li migration number from 0.46 to 0.6, a transport property crucial for suppressing dendrite heterogeneous nucleation [10]. Within solid-state electrolyte systems, Wang Zixuan demonstrated that regulating interfacial stress is critical. When external pressure is appropriately applied, dendrite growth shifts from vertical to lateral expansion; however, exceeding a critical pressure threshold readily induces grain boundary penetration [5].

Leveraging chemical-mechanical synergies, surface coating techniques optimize deposition uniformity. Dong Bangda's team developed MoS_2 functionalized separators exhibiting high ionic conductivity (1.02 mS/cm) with uniform pore distribution. Their two-dimensional layered structure facilitates uniform Li^+ transport while mechanically blocking dendrite penetration [8]. Reportedly, the Li_3N/LiF composite interfacial layer proposed by Hong-Yan Liu's team combines high ionic conductivity with advantages in interfacial energy. Within this composite layer, Li_3N accelerates ion transport while LiF enhances nucleation barriers, enabling dual regulation of deposition morphology [1].

2.2 Regulation of electrolyte interface stability

To suppress lithium dendrite growth, regulating the stability of the electrolyte interface is crucial. The high-concentration electrolyte approach increases the proportion of lithium salts, thereby reconstructing the solvation structure. This significantly reduces the erosion of the interface by free solvent molecules, enabling the formation of a SEI layer enriched with inorganic components such as LiF and Li_2O [1]. The team led by Wang Zixuan also discovered that in all-solid-state electrolyte systems, stress concentration at interfaces causes dendrites to propagate along grain boundaries. Introducing a Li_3N/LiF composite interfacial layer simultaneously enhances ionic conductivity and interfacial energy [5]. Li_3N facilitates ion transport while LiF elevates nucleation barriers, thereby providing dual assurance for interface stability [1].

In engineered interfacial layer design, the SHP developed by Jin Caiyun's team exhibits unique properties. The nanoscale channels formed by twisted polymer chains possess specific confinement effects, enabling selective Li^+ transport and ultimately achieving a Li^+ migration number of 0.6[9]. Dong Bangda's team discovered that functionalized MoS_2 separators, with their uniform pore size distribution, promote uniform Li^+ deposition. Yang Jiayue's team demonstrated through phase-field simulations that the interfacial reaction rate coefficient exhibits a negative correlation with dendrite growth rate. Interfaces with lower reaction rates significantly reduce the range of mechanical stress experienced by dendrite roots [2], laying a theoretical foundation for interfacial kinetic regulation.

Innovations in electrolyte components also yield notable effects. Wang Ce's team proposed COF-1, which reconfigures Li^+ transport pathways through coordination interactions. Its ordered pore structure increased the ion migration number

from 0.46 to 0.6 [10]. Hongang He's team emphasized the critical importance of constructing three-dimensional gradient interface layers in solid-state battery systems. This structure, leveraging both physical contact and chemical bonding, simultaneously reduces interfacial impedance and electron leakage, lowering lithium deposition overpotential by approximately 40% [12].

2.3 Passivation of active sites

One key strategy for suppressing lithium dendrite growth is passivating active sites. Research indicates that defects on the surface of lithium metal anodes exhibit relatively high local electron density, making these areas highly susceptible to preferential Li^+ deposition and triggering heterogeneous nucleation of dendrites [1]. The SHP artificial interface layer developed by Jin Caiyun's team features molecular chains twisted into nanochannels that selectively transport Li+ , increasing the Li+ migration number to 0.6 while effectively stabilizing active sites on the electrode surface [9].

Nitrogen-containing compounds with strong coordination abilities in electrolyte additives have found widespread application in interface passivation. Research by Yang Jiayue's team indicates that nitrocellulose (NC), a macromolecular nitrate ester, possesses nitro functional groups with high electronegativity and nucleophilicity. These groups form stable coordination structures with lithium metal, significantly reducing the occurrence of interfacial side reactions [6]. This approach enhances the uniformity of lithium deposition and improves the cycling stability of all-solid-state batteries.

Surface alloying technology has introduced novel approaches to active site passivation. Constructing a Li-Ag alloy layer on the lithium metal surface modulates charge transport kinetics, promoting synchronous stabilization at the electrolyte interface [13]. The silver component in the alloy layer reduces the overpotential during lithium nucleation, enabling uniform Li^+ deposition over a larger area and preventing localized aggregation of active sites. Similarly, in zinc metal anode research, Jin Cao proposed a $CuZn_5$ alloy interface layer with 97.2% lattice matching. This highly matched epitaxial interface effectively suppresses heterogeneous dendrite nucleation [14]. These studies demonstrate that precise control over the chemical composition and microstructure of interfaces can effectively passivate active sites, thereby laying the foundation for developing lithium batteries with enhanced safety.

2.4 Construction of artificial solid electrolyte interface layers

An innovative strategy to address lithium dendrite issues involves constructing an artificial solid electrolyte interphase (SEI) layer. The SHP developed by Jin Caiyun's team features nano-channels formed by molecular chain distortion, which exhibit unique confinement effects enabling selective Li^+ transport and boosting the Li^+ migration number to 0.6 [9]. Phase-field simulations by Yang Jiayue's team further confirm that an artificial SEI layer with a low interfacial reaction rate coefficient can effectively slow dendrite growth while reducing the mechanical stress range at its root [2].

Regarding material selection, the Li_3N/LiF composite interfacial layer exhibits synergistic effects. Hong-Yan Liu's research indicates that Li_3N possesses high ionic conductivity pathways that accelerate Li^+ transport, while LiF enhances nucleation barriers. Together, they ensure interfacial stability through dual mechanisms [1]. The team led by Wang Zixuan identified a composite interfacial layer with unique properties that simultaneously reduces interfacial impedance and electron leakage, lowering the lithium deposition overpotential by approximately 40% [13]. The mechanical properties of engineered SEI layers must align with electrode volume changes. Excessively high modulus causes interfacial delamination, while excessively low modulus fails to suppress dendrite penetration. Dong Bangda's team developed MoS_2 functionalized separators featuring uniformly distributed pore sizes. These separators effectively prevent dendrite penetration through mechanical barrier effects [8], embodying a balanced design philosophy integrating mechanical and electrochemical performance.

Regarding construction methods, in-situ reaction and pre-deposition techniques each possess distinct characteristics. Due to the high electronegativity of nitro functional groups, nitrocellulose (NC) forms stable coordination structures with lithium metal. This enables the in-situ formation of an interface layer with ion homogenization capabilities during cycling [6]. The Li-Ag alloy layer fabricated via physical vapor deposition (PVD) technology regulates charge transport kinetics. Achieving an exceptional lattice matching degree of 97.2% during epitaxial growth, it effectively suppresses heterogeneous dendrite nucleation [14]. In solid-state battery systems, the three-dimensional gradient interface layer proposed by Hongang He successfully overcomes the resistance and stress concentration issues arising from solid-solid contact [12]. Overall, to achieve a satisfactory artificial SEI layer, it must possess chemical stability, mechanical adaptability, and dynamic self-healing capabilities.

2.5 Electrode surface microstructure design

In suppressing lithium dendrites, designing electrode surface microstructures represents a cutting-edge strategy. This approach enables precise control over the electrode's geometric shape and physical properties, fundamentally altering Li^+

deposition behavior. The design of three-dimensional porous current collectors significantly increases specific surface area, thereby substantially reducing local current density. Research by Lin Yu's team further demonstrates that introducing nanoscale pore structures onto copper current collectors can reduce lithium nucleation overpotential by approximately 60%, significantly promoting uniform deposition[7]. Such structures provide numerous nucleation sites, preventing surface charge aggregation.

From the perspective of micro-morphology regulation, biomimetic structural design offers unique advantages. Phase-field simulations conducted by Yang Jiayue's team revealed that electrode surfaces with fractal characteristics can utilize multi-scale effects to disperse electric field intensity. This keeps the Li^+ deposition Damköhler number within an optimal range, thereby suppressing dendrite longitudinal growth[2]. The MoS_2 functionalized separator developed by Dong Bangda employs a micro-nano composite structure that simultaneously provides mechanical barriers and ion homogenization, achieving synergistic dendrite suppression.

From another perspective, key aspects of microstructure design also involve regulating surface wettability. Jin Caiyun's team proposed SHP, while Wang Zixuan discovered that constructing a Li-Ag alloy layer on the lithium metal surface can modulate interfacial energy distribution. This alloying approach, integrating chemical modification with microstructure control, offers novel insights for interface design.

The limitations inherent in traditional homogeneous materials have been successfully overcome through gradient structure design. The three-dimensional gradient interface layer proposed by Hongang He's team and the surface nucleation and diffusion model proposed by Wen Xinyi's team demonstrate that precisely controlling the microstructure of electrode surfaces requires simultaneous consideration of multiple aspects—including geometric morphology, wettability characteristics, and mechanical properties—and the synergistic optimization of multiple parameters.

3 Summary and outlook

3.1 Conclusion summary

Dendrite suppression strategies and interfacial chemistry in lithium batteries hinge on achieving a synergistic balance between electrochemical kinetics and mechanical stability. Uneven ion distribution on electrode surfaces and defects in the SEI film can trigger lithium dendrite growth. Optimizing electrolytes, employing three-dimensional current collectors, and fabricating engineered SEI films can enhance lithium deposition conditions. Research indicates that phase-field simulations conducted by Yang Jiayue's team demonstrate relatively low interfacial reaction rate coefficients positively influence slowing dendrite growth rates [2]. By regulating the solvation structure of high-concentration electrolytes, a dense interfacial layer was constructed [1]; Jin Yun's team achieved a Li^+ migration rate of 0.6 through their SHP artificial interfacial layer [9]. In solid-state electrolytes, the Li_3N/LiF composite interfacial layer reduced deposition overpotential by 40% [1]. Three-dimensional current collectors help reduce local current density, while biomimetic structures can disperse electric field strength [2]. Wang Zixuan's team noted that external pressure must precisely match material properties [5]. Current challenges include unclear interfacial reaction mechanisms and imperfect fabrication processes [7]. Future efforts should focus on integrating multiscale characterization with machine learning-assisted design to explore synergistic optimization strategies for gradient modulus interfacial layers [12].

3.2 Future application directions (Outlook)

In the future, the development trend of lithium battery interfacial chemistry will move toward multidimensional cross-integration, leveraging machine learning for assisted design to potentially break through research bottlenecks. Utilizing deep learning algorithms and establishing material databases can enhance the development efficiency of high-performance interfacial materials. According to Yang Jiayue's research [2], low interfacial reaction coefficients play a role in suppressing dendrite growth, providing a basis for model optimization. In solid-state batteries, structures like the bistable architecture proposed by Hongang He's team [12] —a three-dimensional interfacial layer with gradient modulus—are poised to become a mainstream development direction. Wang Zixuan suggests verifying the connection between interfacial stress and dendrite growth [5]. In the field of smart interfacial materials, the SHP polymer adopted by Jin Caiyun's team demonstrates potential for self-healing [9]. Achieving large-scale production requires breakthroughs in low-cost processes. For instance, the MoS_2 functionalized separator developed by Dong Bangda's team demonstrates industrial feasibility. Future efforts should focus on synergistic interface-bulk optimization to establish multi-level stable architectures, thereby advancing the development of high-safety batteries with energy densities reaching 50 Wh/kg.

3.3 Technical challenges and potential breakthrough pathways

Two major challenges exist in the field of lithium battery interface regulation: elucidating dynamic mechanisms and

achieving large-scale preparation. Research by Yang Jiayue's team indicates that low reaction rate coefficients can suppress dendrite growth; however, the lack of atomic-level observation methods means artificial SEI design must rely on empirical approaches [2]. According to Hongang He, solid-solid interfaces in solid-state batteries present a contradiction between chemical bonding and physical contact [12], which exacerbates the non-uniformity of three-dimensional current collector structures [12]. Wang Zixuan's team developed an interface stress and force-electrochemical coupling model for dendrite growth [5]. Jin Caiyun's team proposed dynamic adaptive interfacial layers (e. g., SHP), which regulate ion transport through conformational changes to address interfacial delamination [9]. Regarding fabrication, Dong Bangda's team demonstrated the feasibility of preparing functionalized separators via simple coating methods [8]. Future efforts should focus on developing cost-effective techniques like solution polymerization and leveraging machine learning for material property prediction. These innovations will propel interface regulation from the laboratory to industrialization.

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