

Enhancing Electrochemical Kinetics in Lithium-Ion Batteries with Hollow and Porous Si Anodes

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Presentation Keywords: lithium-ion batteries, anode, silicon nano-quill, high current rate cycling, fast charging

This research addresses the dual challenges of escalating energy demands and the limitations of current lithium-ion battery (LIB) anodes by pioneering a novel synthesis methodology for mesoporous silicon materials. Utilizing bio-renewable cellulose nanocrystals (CNCs) as a sacrificial template, our team has developed a cost-effective, scalable, green approach to create 3-dimensional silicon nano-quills (SiNQs). The SiNQ anodes, characterized by their unique porous and hollow nanostructures, offer superior battery performance at high current rates. We employed a unique testing scenario where the electrodes underwent three cycles at a lower current rate (0.1C) followed by ninety-seven cycles at a high rate (2C), repeated five times for 500 cycles. Initially, the battery displayed a reversible discharge capacity of 1.32 mAh cm⁻² at 0.1C. Remarkably, after undergoing cycles at the higher 2C rate, the battery's capacity showed notable recovery during the subsequent 0.1C cycling intervals. In each subsequent interval, the capacity values achieved were 1.46, 1.39, 1.33, and 1.30 mAh cm⁻², respectively.

This behavior underscores the potential of SiNQ-g as a viable material for fast-charging battery applications. Furthermore, this research delves into the complex electrochemical dynamics within these novel anodes. Through detailed electrochemical analysis using Cyclic Voltammetry (CV), we examine lithium diffusion and phase transformations within the electrode materials. A particular focus is on the SiNQ anodes, where their specific surface area and structural attributes significantly influence the electrochemical behavior, especially at higher scan rates. This unique behavior is analyzed using a combination of experimental data and theoretical models, highlighting the potential of SiNQ-based electrodes for fast-charging applications. The study not only advances the synthesis of mesoporous silicon materials but also provides an insightful understanding of the electrochemical mechanisms at play in next-generation LIB anodes. The currently existing CV models (and the methodology to distinguish between capacitive and diffusive contributions) assume (a) semi-infinite diffusion and (b) the presence of both oxidized and reduced species of the redox couple present within the electrolytic solution, and neither of these assumptions are valid for lithium-ion batteries. Our newly developed CV model addresses

some of these fundamental concerns for cases where the ionic diffusion within the solid electrode particles is the rate-limiting step.

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Multiphysics modeling of hybrid thermal management systems for Li-ion battery modules

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Presentation Keywords: Finite element method, Batteries, Thermal Management Systems, COMSOL, Thermal interfaces

Introduction: Over the last decade, with the advance of lithium-ion battery (LIB) with its enhanced performance in cycle life and energy density, electric vehicles (EV) have become one of the dominant sectors in the industry and research, fostering significant advancements and breakthroughs. Despite its growth potential, heightening concerns about battery thermal issues have drawn the great attention of researchers all across the world. Research indicates a significant temperature increase of 10-20 °C on the battery surface when transitioning from a 1C to a 4C discharge rate, posing efficiency challenges and potential degradation risks, including the risk of thermal runaway. Consequently, extensive efforts have been directed towards developing Battery Thermal Management Systems (B-TMS), encompassing various approaches such as air and liquid cooling mechanisms, innovative battery pack designs, and the integration of phase change materials (PCMs). A highly efficient B-TMS demands the fabrication of an electrically insulating, mechanically stable platform with efficient thermal distribution. In this study, we performed Multiphysics modeling of actively cooled B-TMS with polymer-2D material (graphene and BN) composites serving as the thermal interface materials (TIMs).

Methodology

With material parameters derived through experimental investigation, we employ the 3D finite element method (FEM) to model the 3S2P configuration of 21700 batteries packed with Al serpentine tubes (with and without TIMs). By incorporating heat transfer and laminar flow as physical interfaces with the battery pack module, simulation is carried out for different scan rates and coolant flow rates to obtain T_{max} and ΔT between different cells in the module.

Results

With boundary condition of $T=T_0$ at the outer surface and $-n \cdot q = \frac{P_0}{A}$ at the inner surface of Al tubing, the temperature profile is mapped for coolant rate 0.1 to 0.8 m/s. Here P_0 is the heat rate. In the preliminary studies, T_{max} showed an average decline of ~ 3.4 K across the simulated coolant flow rate.

Conclusion

In summary, we computationally modeled the battery pack with cells thermally interfaced into a serpentine cooling system using polymer-2D material composites. The charge-discharge studies for different C rates estimate the heat generated, which is then used to analyze the temperature profile across the pack for different controlling parameters for the cross analysis with

experimental results. We found that 10-30 wt. % polyimide-graphene/BN composites showed a low ΔT compared to acrylic plastic and polyimide.

Development of a GITT model for Si-embedded Carbon-cloud electrode

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Keywords: Si-embedded carbon cloud, diffusion coefficient, galvanostatic intermittent titration technique, two phases, equilibrium potential

The huge demand for high-capacity, energy-dense, low-cost, and environmentally friendly lithium-ion (Li^+) batteries for energy storage devices has led to intense research for new electrode materials. Silicon (Si) is a promising anode material because it can address the requirements mentioned above. Although the concept of Si-Li cell looks attractive, it shows poor performance due to insufficient space in the electrode to accommodate the volume change of Si during lithiation/delithiation. At room temperature, slow diffusion of Li^+ in Si, low electronic conductivity of Si, and slow kinetics pose challenges. To mitigate such problems, we embedded Si nanoparticles in a porous carbon cloud. Si-based electrodes undergo phase transformation and massive volume changes during lithiation/de-lithiation. This leads to the generation of mechanical stress-strain, which affects lithium ion diffusion. The carbon cloud also contributes to charge storage, affecting the diffusion of lithium ions within the electrode particles. While electrode particle level galvanostatic intermittent titration technique (GITT) models exist for intercalation and phase-transformation electrodes, they do not account for volume changes and the consequential generation of mechanical stress and strain. Therefore, we developed a novel GITT model to study the Li^+ diffusion in silicon-embedded carbon cloud electrodes. Our model accounts for phase changes in Si, volume changes in silicon, related mechanical stress-strain, and the diffusion of Li^+ ions from the electrolyte to the Si nanoparticles via the carbon cloud. Our physics-based analytical model may be used to mass transfer within Si-embedded carbon cloud electrode particles as a function of the state of charge-discharge. The diffusion coefficient of lithium ions within both phases of Si can be obtained by fitting the obtained theoretical concentration profiles with the experimental data.

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