Computational Modeling of Dendrite Growth: A Key Challenge in Lithium Battery Development

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ABSTRACT

Lithium metal is a promising anode for next-generation batteries due to its high specific capacity. However, repeated lithium plating and stripping during cycling is unstable, often leading to dendrite formation, poor battery performance, and short-circuit risks. The dendrite growth is a multiscale, complex process, spanning from molecular-scale electrolyte decomposition to macroscale structures, and can develop into various morphologies, such as needle-like, mossy, or fractal structures. The thin solid electrolyte interphase (SEI), which exists between the anode and electrolyte, is widely believed to be a key factor determining lithium plating stability. Despite its critical role, the SEI is often oversimplified in analytical models due to its nanometer-scale thickness. As a result, several stability criteria, such as limiting current density and Sand's time, frequently fail to provide accurate predictions of experimental dendrite behaviors. To improve our understanding of lithium dendrite growth, we developed a phase-field model to simulate the dendrite growth during plating instability, which incorporates the electrochemical reactions, lithium ion diffusion, and interfacial evolution. Our results show that, despite its nanometer thickness, SEI properties, including ion transport, evolution, and fracture, play a critical role in plating stability.