Modeling solid-electrolyte interphase formation on silicon interfaces

Lithium-ion batteries combine good long-term stability and performance. These properties have made Lithium-ion batteries the benchmark energy storage for hand-held electronics and electric vehicles. Nevertheless, there is an industrial urge to further push the technology towards higher capacities and longer battery life. Increasing the lifetime of Lithium-ion batteries is currently a fundamental challenge for battery research. Due to the growth of a solid-electrolyte interphase (SEI) during storage and cycling, capacity is irreversibly lost.

Silicon anodes are a promising approach for further increasing the capacity of Lithium-ion batteries, as they show the tenfold theoretical specific capacity of the currently used graphite anodes. However, the SEI growth is even more severe for silicon anodes: large volume expansions of ~300% exert high mechanical stresses and fracture the SEI. The resulting cracks subsequently expose the pristine electrode leading to SEI reformation and thereby continuous capacity decrease.

In order to further understand SEI growth, our group developed a model describing SEI growth on graphite during storage [1-4]. Additionally, a thermodynamical framework was developed to describe the coupling of different physical effects [5]. Based on these theories, we include mechanical stresses and study their impact on SEI stability and growth during battery operation. Understanding these relationships identifies critical operating conditions and aid in the design of new electrodes. Thereby, batteries with higher capacity and long-term stability can be developed.

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