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Degradation and life prediction of Li-ion cells

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The electrification of the drivetrain is crucial to solve our energy problems and fill the gap to sustainable and zero emission mobility. We are now within reach of mass-marketed vehicles using Li-based batteries. Full engineering analysis of batteries and battery systems must be regularized, and engineering development is needed to allow creation of products and tools for integration of battery systems into vehicles. Electric Vehicles (EV) and Hybrid Electric Vehicles (HEV) face significant battery-related challenges, including limited driving range and high battery cost resulting from the capacity fade of batteries during usage. The prediction of capacity fade and lifetime of batteries is important for cell design, determination of the optimal operation condition and control, and cell maintenance, and eventually the successful implementation of HEVs and EVs. Various mechanisms contribute to capacity fade, especially in large format cells which use multiple-material electrodes to enhance the performance. An integrated approach considering different aspects of the fading mechanisms is necessary. In this talk I will present some of our recent works on modeling the fading mechanisms in Li-ion batteries together with experimental investigations. Specifically, I will focus on those mechanisms that are not well understood before, such as side-reaction coupled behaviors, stress evolution in active material particles due to coupled phase transition and intercalation, facture of active material particles, ion diffusion and percolation, dissolution of active materials, heat generation under various operational and environmental conditions, and effects of face pressure on cell performance. We have developed a life prediction framework that integrates multiple physics across different scales — including electrochemical, transport, thermal, mechanical and thermodynamic processes. Assisted with experimental measurements, we are incorporating realistic three dimensional electrode microstructures in our models for high fidelity simulation and prediction.

Keywords: Li-ion battery; Capacity fade; Side reaction; Multiphysics; Modelling

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锂离子电池的退化与寿命预测

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动力传动系统电气化对于解决我们的能源问题，实现可持续发展和零排放是至关重要的。我们现在正步入基于锂电池的电动汽车实现大规模市场化的关键时期。这对于建立锂电池和电池系统完整全面的分析方法，以及发展将电池系统集成到车辆上的系统模拟工具，提出了迫切要求。电动汽车和混合动力汽车面临着与电池相关的严重挑战，包括有限的续航里程及电池在使用过程中容量衰减导致的高电池成本。电池容量衰减及寿命预测对于电池单元设计、确定电池最佳的工作状态和优化控制、电池的有效维护、及最终成功规模化实现混合动力汽车和电动汽车非常重要。多种机制导致了锂离子电池，特别是应用多材料电极以提升性能的大型锂离子动力电池的容量衰减。因此，整体考虑多种衰减机制并建立统一的分析方法十分必要。这里我将介绍我们近期在锂离子电池退化机制的模拟及实验研究方面的一些工作。具体来说，本报告将着重于那些目前尚未很好理解的机制，如耦合了副反应的电池内部过程、相变与嵌入引发的活性材料颗粒的应力、活性材料颗粒的断裂与剥落、离子扩散与渗透、活性材料溶解、多种工作和环境条件下的热生成过程、及表面压力对电池性能的影响。我们建立了一个预测电池寿命的框架，整合了不同尺度下的多物理过程：包括电化学、输运、热、机械及热力学过程。同时我们将实验测量的电极真实三维微结构应用于模型以实现更精确的模拟和预测。

关键词：锂离子电池；容量衰减；副反应；多物理场；模拟