MATERIALS ENGINEERING SEMINAR

"Physics Based Modeling of Degradation in Lithium-Ion Batteries"

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ABSTRACT

A generalized physics-based modeling framework is presented to analyze: (a) the effects of temperature on identified degradation mechanisms, (b) interfacial debonding processes, including deterministic and stochastic mechanisms, and (c) establishing model performance benchmarks of electrochemical porous electrode theory models, as a necessary stepping stone to perform valid battery degradation analyses and designs. Specifically, the effects of temperature were incorporated into a physics-based, reduced-order model and extended to a $LiCoO_2$-graphite 18650 cell. Three dimensionless driving forces were identified, controlling the temperature-dependent reversible charge capacity. The identified temperature-dependent irreversible mechanisms include homogeneous SEI, at moderate to high temperatures, and the chemomechanical degradation of the cathode at low temperatures. Also, debonding of a statistically representative electrochemically active particle from the surrounding binder-electrolyte matrix in a porous electrode was modeled analytically, for the first time. The proposed framework enables to determine the space of C-Rates and electrode particle radii that suppresses or enhances debonding and is graphically summarized into performance-microstructure maps where four debonding mechanisms were identified and condensed into power-law relations with respect to the particle radius. Finally, in order to incorporate existing or emerging degradation models into porous electrode theory (PET) implementations, a set of benchmarks were proposed to establish a common basis to assess their physical reaches, limitations, and accuracy. Three open-source models: dualfoil, MPET, and LIONSIMBA were compared, exhibiting significant qualitative differences, despite showing the same macroscopic voltage response, leading to different conclusions regarding the battery performance and possible degradation mechanisms of the analyzed system.

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Place: ARMS 1028 or via Webex:
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