Contribution ID: **497** Type: **Poster (+) Presentation**

Modeling lithium diffusion in battery cathodes considering chemo-mechanically induced damage

Monday, 31 May 2021 19:35 (1 hour)

This talk will present a 3D, continuum-level damage model for simulating Lithium diffusion within generated $Li_xNi_{0.5}Mn_{0.3}Co_{0.2}$ (NMC 532) secondary cathode particles. The primary motivation of the particle-level model is to inform cathode-particle design and determine charging profiles that reduce cathode fracture. The model considers NMC 532 secondary particles containing an agglomeration of anisotropic, randomly oriented grains. The model predicts that secondary-particle fracture is primarily due to non-ideal grain interactions with slight dependence on high-rate charge demands. The model predicts that small secondary-particles with large grains develop significantly less damage than larger secondary particles with small grains. Finally, the model predicts most of the chemo-mechanical damage accumulates in the first high-rate cycles. This chemo-mechanical "damage saturation" effect indicates that initial secondary-particle fracture occurs within the first few cycles, while long-term cathode degradation is not solely chemo-mechanically induced.

Time Block Preference

Time Block C (18:00-21:00 CET)

References

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