MATERIALS ENGINEERING

SEMINAR

"Data Driven Microstructural Design of Porous Electrodes"

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ABSTRACT

Porous lithium ion battery (LIB) electrodes are comprised of electrochemically active material particles that store lithium and a surrounding conductive binder, liquid electrolyte, carbon black mixture that facilitates ionic and electronic transport. Typically, lithium diffusivity is several orders of magnitude smaller in the active material as compared to the surrounding electrolyte, making the electrode microstructure a governing factor in determining the balance between its lithium storage capacity and transport rate. Here, the effects of microstructure on the performance of LIBs are systematically analyzed at three length scales - the single particle length scale, the spatially resolved multiple particle length scale, and the porous electrode layer (homogenized) length scale. At the single particle length scale, a thermodynamically consistent variational framework is presented to examine the effects of crystallographic anisotropy, crystallographic texture, grain size, and grain morphology on the $LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$ (NMC111) chemistry. The theory was extended to the spatially resolved multiple particle length scale and the porous electrode layer length scale to explain the microstructural origin of experimentally observed instances of apparent phase separation in NMC111. At the electrode length scale, a data driven framework is presented to evaluate the electrochemical performance of a wide range of particle morphologies and battery architectures. Specifically, microstructural characteristics of 53 356 microstructures are assessed, and strategies to optimize electrode design parameters such as active particle morphology, spatial orientation, electrode porosity, and cell thickness are presented.

Place: https://purdue.webex.com/purdue/j.php?MTID=md76713504103add582720df99d2bc8cb
Time: Tuesday, Nov 2, 2021 12:00 pm | 1 hour | (UTC-04:00) Eastern Time (US & Canada)
Meeting number: 2622 861 5362
Password: e2jCJ26N6b4

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