Tailing the Morphological Evolution of Interfaces in Lithium Battery Materials

Abstract: Various types of interfaces exist in materials for lithium storage materials, which include but are not limited to electrode/electrolyte interfaces, phase boundaries between lithiated and delithiated phases, and grain boundaries. Interfaces in Li battery electrodes often exhibit intricate morphological changes upon electrochemical cycling, which are coupled with charge transport and have significant impact on electrode properties. Two examples will be presented in this talk to demonstrate that tailoring interface morphology and its evolution offers a useful strategy to enhance the performance and reliability of lithium battery materials. We first discuss our mesoscale modeling study on lithium iron phosphate olivine (LiFePO4), an important cathode material for Li-ion batteries. Through phase-field simulations, the important role of coherency stress on the stability and orientation of phase boundary in LiFePO4 is revealed. Based on this understanding, we show that an order of magnitude increase in rate capability can be achieved through the control of particle morphology. The second example focuses on Si anodes. Upon Li insertion, crystalline Si undergoes an amorphous phase transition accompanied by a >300% volume expansion. Using an interface-tracking model, we show that the anisotropic mobility of the phase boundary between the crystalline and amorphous phases results in anisotropic swelling behavior, which gives rise to high tensile strain concentration and crack initiation on electrode surface. Accordingly, a novel strategy is developed to mitigate lithiation-induced fracture by morphological design of Si structures, the effect of which is demonstrated experimentally.
**Bio of Dr. Tang:** Ming Tang is an assistant professor of Materials Science and NanoEngineering at Rice University. He obtained his B.S. and M.S. from Shanghai Jiao Tong University, China, and a Ph.D. degree in Materials Science and Engineering from MIT. He was a Lawrence Postdoctoral Fellow and then Staff Scientist at the Lawrence Livermore National Laboratory (LLNL), where he led efforts on mesoscale modeling of lithium-ion batteries and microstructural evolution in materials under extreme conditions. Before joining Rice, he also worked at the Shell Technology Center Houston as a Materials & Corrosion Research Engineer, where he focused on applying materials knowledge and technologies to solve practical problems in the oil & gas industry.

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