A MULTIPHYSICS MODEL FOR THE STRESS ANALYSIS OF LITHIUM ION BATTERY

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KEYWORDS

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ABSTRACT

High capacity materials can dramatically improve the energy density of the lithium ion batteries (LIBs). To utilize these materials in LIBs, however, is very challenging. A high Li storage capacity is often accompanied with large volume variation and high stress in the materials. For example, for anode materials, silicon (Si) offers the highest Li storage capacity besides the pure Li itself. Each Si atom can accommodate up to 4.4 Li atoms, providing a gravimetric capacity over 3500 mAh/g and a volumeric capacity over 8300 mAh/ml. These values are one order of magnitude higher than those of graphite. Nevertheless, the lithiation of Si is accompanied with more than 300% volume variation. The large volume fluctuation induces high cyclic stresses in the active material and can cause fracture. As the active materials are not stand alone but connect or in contact with other components, the volume fluctuation may induce stresses and cause failure in other components and regions such as the binder, and the interfaces between binder/active material and active material/current collector. All these events can lead to loss of electrical contacts in local areas and rapid capacity fading of the battery. The volume variation is also a serious concern in the design of battery packs.

Mechanics is an important aspect in the design of LIBs with high capacity electrodes. Numerical simulations will be imperative in such design. Although simulations have been widely used in stress analysis of various engineering structures, models that incorporate Multiphysics are still lacking. To authors' best knowledge, computation tools that are capable of performing stress analysis of LIBs with high capacity battery electrodes with battery cycles have not been reported.

In previous works, we have developed a series of Multiphysics, models for the stress analysis of $Li_xC_6Li_y$|LiPF6(EC/DMC)|Mn_2O_4 cell[1-4], including a multiphysics micro-structure resolved (MMR) model[4] shown in Fig.1. The MMR model consists of two sub-models: Electrochemical and Stress. The species transport and battery kinetics are computed in Electrochemical sub-model. The deformations and stresses are computed in Stress sub-model. The two sub-models are coupled directly through the Li concentration and deformation fields. The model was implemented in COMSOL. This model is capable of revealing the stress and deformation in each battery components with cycles.

In this talk, we will present the recent development in MMR model for LIBs with Si anode.

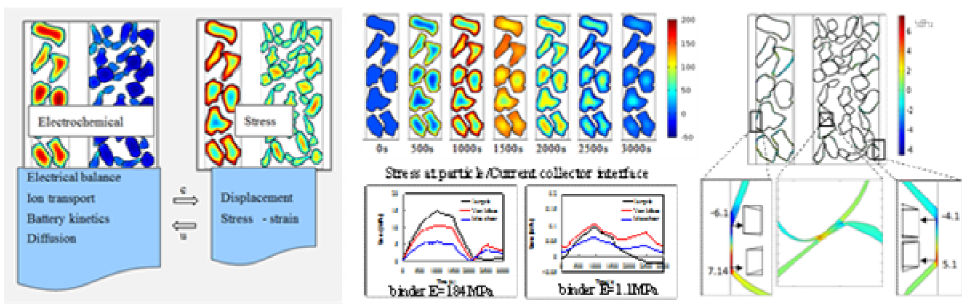

Fig.1 MMR model for a $Li_xC_6Li_y$|LiPF6(EC/DMC)|Mn_2O_4 cell. The major components from left to right are Cu current collector/anode/separator/ cathode/Al current collector. Active particles and binder are modeled explicitly in the two electrodes. Clockwise from left: two sub-models and their coupling; the stress evolution in active particles in anode for a galvanostatic discharge-charge cycle at 2C: discharge (0-1000s), open circuit period (OCP) (1000s-1500s), charge (1500s-2500s), and OCP (2500s-3000s); the shear stress in binder at different interfaces; the evolution of the stresses at the particle/Cu current collector interface for two binders with modulus E=184 and E=1.1MPa.

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