2D Micro-Structure Resolved Model for Li-Ion Battery

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High capacity rechargeable lithium-ion battery is considered as a promising storage device for portable electronic devices and electric vehicles, etc. High capacity anode materials such as Silicon and Tin experience large volumetric changes during charge/discharge cycling in battery cells. Silicon's volume changes by 300% upon insertion and extraction of lithium[1]. Large cyclic deformation often leads to particle fracture, mechanical failure and delamination at particle-binder, particle-current collector interfaces, which results in pulverization and capacity fading. The loss of electrical connectivity is a major mechanism of capacity fading[2]. Also, this large volume expansion/contraction forces large pressure to separator, which cause the large stress and strain during this process and may lead to serious thermal event due to separator failure. Large cyclic deformation may also cause the porosity and tortuosity of an electrode vary instead of being constants, which is in addition to the inhomogeneity induced variation in local tortuosity. To model the battery performance accounting for these behaviors requires a model with realistic microstructure representation and considers the multiphysics involved in these phenomena.

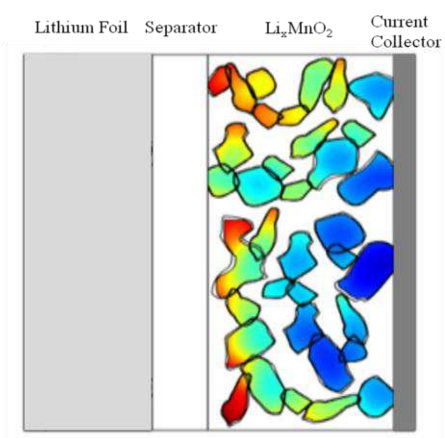

Figure 1 Li concentration in micro-structured lithium magnesium oxide electrode in half cell model.

This paper presents a multiphysics battery model with micro-structure resolved capability. At the current stage, the model is used to investigate the stresses in electrode matrix along with battery cycles. A 2D microstructure resolved model of lithium magnesium oxide half cell is developed. The relationship between local tortuosity and the concentration polarization of Li^+ in electrolyte is investigated. The stress evolution in the active particle during battery charge and discharge is studied. The concentration variations due to particle sizes and morphology are examined and compared.

References:

1. Ge, M., et al., Porous Doped Silicon Nanowires for Lithium Ion Battery Anode with Long Cycle Life. Nano Letters, 2012. **12**(5): p. 2318-2323.
2. Boukamp, B.A., G.C. Lesh, and R.A. Huggins, All-Solid Lithium Electrodes with Mixed-Conductor Matrix. Journal of The Electrochemical Society, 1981. **128**(4): p. 725-729.