Influence of Morphology and Microstructure on the Lithium-Ion Battery Electrode Damage Behavior

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Electrode microstructures play a major role in the determination of performance and life span of a battery¹. Most commercial battery electrodes consist of four phases, active material, conductive additive, binders and electrolyte (see ²⁻⁴). Active materials are responsible for hosting Li ions. Transportation of Li ions occurs through the electrolyte. Because of the presence of conductive additives and binders, entire surface areas of active particles do not have access to the electrolytes. Hence directional lithiation (or delithiation) happens to (or from) the active particles. Depending on the crystal microstructure, anisotropic diffusion of Li ions is also possible inside the particles. Microstructural grain-grain boundary orientation introduces irregularities in concentration gradient, which can impact generation and fracture of active particles⁵. stress



Figure 1: (a) Two dimensional cross sectional image of a representative electrode microstructure. (b) Small section of a representative electrode microstructure adopted to demonstrate the impact of Li diffusion on active particles. Presence of binders restricts the access of electrolyte to the active particles. Concentration profile after delithiation at 6C for 500s has been plotted in the figure.

In our previous study a model was developed to capture the diffusion induced fracture in a single spherical active particle⁶. The model has been extended to incorporate the Li ion diffusion profile in realistic electrode microstructure. Diffusion induced fracture has also been captured successfully. Degradation in capacity due to fracture of active particles in an actual electrode microstructure will be analyzed in this study.



Figure 2: Diffusion induced fracture in a representative electrode microstructure under directional delithiation at 6C. (a) Time, t = 250s. (b) Time, t = 500s.

References

- 1. P. Barai, S. Simunovic, and P. P. Mukherjee, *in* "Proceedings of the ASME International Mechanical Engineering Congress and Exposition (IMECE)", Houston, 2012.
- G. Liu, H. Zheng, X. Song, and V. S. Battaglia, J Electrochem Soc, 159 (3), A214-A221 (2012).
- 3. S. Xun, X. Song, V. Battaglia, and G. Liu, *J Electrochem Soc*, **160** (6), A849 - A855 (2013).
- 4. M. Zhu, J. Park, and A. M. Sastry, *J Electrochem Soc*, **158** (10), A1155-A1159 (2011).
- 5. W. H. Woodford, W. C. Carter, and Y.-M. Chiang, *Energy and Environmental Science*, **5** 8014 8024 (2012).
- 6. P. Barai and P. P. Mukherjee, *J Electrochem Soc*, **160** (6), A955 A967 (2013).