11th World Congress on Computational Mechanics (WCCM XI)
5th European Conference on Computational Mechanics (ECCM V)
6th European Conference on Computational Fluid Dynamics (ECFD VI)
July 20 - 25, 2014, Barcelona, Spain

Phase Transformation and Fracture During Lithiation in $LiFePO_4$ Electrodes

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Key Words: *Phase-Field, Fracture, Phase-Transformation, Energy Systems.*

Due to the growing demand of lithium-ion batteries for use in everything from cell phones to electric vehicles, there is a pressing need for a better understanding of the phenomena that limit battery life. One such mechanism that has been linked to the degradation in charging capacity of lithium-ion batteries is electrode fracture. It has been shown that fracture in an electrode during lithium extraction/insertion can be linked to large volume changes and high internal strains at the interface of the two-phase LiFePO4/FePO4 structure [1]. To better understand these issues this work develops a new model that couples phase transformation and fracture in lithium-ion batteries. The phase transformation is simulated using the recently developed reaction-limited phase-field model for Li-ion intercalation in single nanoparticles [2] while the fracture is modelled using the phase-field fracture approach [3]. Distributions of lithium concentration during charge/discharge cycles and the high stress that develops at the phase boundary in the electrode is presented. Furthermore, the situations in which fracture can arise and propagate are discussed. The model has shown the ability to capture the inhomogeneous distribution of lithium in an electrode and the subsequent fracture initiation and propagation.

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