Society of Engineering Science 51st Annual Technical Meeting

1–3 October 2014

Purdue University, West Lafayette, Indiana, USA

Classifying the mechanisms of electrochemical shock in ion-intercalation materials

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ABSTRACT

"Electrochemical shock" – the electrochemical cycling-induced fracture of materials – contributes to impedance growth and performance degradation in ion-intercalation batteries, such as lithium-ion. Using a combination of micromechanical models and acoustic emission experiments, the mechanisms of electrochemical shock are identified, classified, and modeled in targeted model systems with different composition and microstructure. A particular emphasis is placed on mechanical degradation occurring in the first electrochemical cycle. Three distinct mechanisms of electrochemical shock are identified, and a fracture mechanics failure criterion is derived for each mechanism. In a given material system, crystal symmetry and phase-behavior determine the active mechanisms. A surprising result is that electrochemical shock in commercial lithium-storage materials occurs by mechanisms that are insensitive to the electrochemical cycling rate. This fundamental understanding of electrochemical shock leads naturally to practical design criteria for battery materials and microstructures that improve performance and energy storage efficiency. These microstructure and crystal chemical design criteria are demonstrated experimentally for spinel materials such as $LiMn_2O_4$ and $LiMn_{1.5}Ni_{0.5}O_4$. A case study of $LiMn_{1.5}Ni_{0.5}O_4$ is presented, in which small changes in composition that have negligible impact on electrochemical properties induce a significant change in phase behavior that allow electrochemical shock at relevant electrochemical cycling rates to be avoided. Although lithium-storage materials are used as model systems for experimental study, the physical phenomena are common to other ion-intercalation systems, including sodium- and magnesium-storage compounds.