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Generation of stress in the storage particles of lithium-ion batteries

McMeeking, Robert, rmcm@engineering.ucsb.edu, UC Santa Barbara

ABSTRACT

Models are developed for the transport of lithium (Li) ions in the electrolyte of Li ion batteries, their diffusion through storage electrode particles, and their kinetics through the surface of the particles between the electrolyte and the particles. As a consequence of the Li ion intercalating in the storage particles, their lattice swells, leading to elastic stress when the concentration of Li ions in the particles is not uniform. The models of transport are based on standard concepts for multicomponent diffusion in liquids and solids, but are not restricted to dilute solutions, or to small changes in the concentration of the diffusing species. In addition, phase changes are permitted during mass transport as the concentration of Li varies from the almost depleted state of the storage particle to one where the material is saturated with its ions. The elastic swelling and shrinkage may involve very large dilatations, which can be allowed for in the formulation of the model. Thus, the models can be suitable for storage particle, where the amount of Li can vary by large amounts depending on the state of charge, for staging as observed in the storage process in graphite, for the enormous swelling that takes place when silicon is used for storage, and for electrolytes in which the concentration of Li ions is high. The model is used to compute the processes of charging and discharging the battery to assess the parameters that influence the development of stress in the storage particles, and to deduce the likelihood of fracture of the storage particle material. The objective is to assess designs of porous electrode microstructures that permit rapid charging and discharging, but obviate the likelihood of fracture and other mechanical damage that limit the performance and reliability of the battery.