



The Generation of Stress in the Storage Particles of Lithium-Ion Batteries

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Models are developed for the transport of Li ions in the electrolyte of lithium 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 multi-component 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 lithium 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.

Keywords: lithium-ion; battery; stress; storage-particle



锂离子电池存储颗粒中的应力产生

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建立模型用于描述锂电池电解质中锂离子的传输，其通过存储电极颗粒的扩散，和介于电解质和颗粒之间颗粒表面的动力学。由于锂离子插层，存储颗粒晶格膨胀，这样当锂离子在颗粒中的浓度不均匀时会导致弹性应力。传输模型是基于标准的液体和固体中多组分扩散的概念，但不局限于稀溶液，或扩散物种浓度的微小变化。此外，从存储颗粒材料处于几乎离子耗尽的状态，到材料处于离子饱和状态，这之间由于锂的浓度变化，在物质传输过程中产生的相应相位变化是允许的。弹性膨胀和收缩可能涉及非常大的膨胀，这在模型推导中也是允许的。因此，本模型适用于存储颗粒，其中的锂离子量可以根据不同的充电状态而有很大变化，适用于石墨存储过程中观察到的分段现象，适用于当硅用于存储时发生的巨大肿胀，也适用于锂离子的浓度高的电解质。该模型用于评估电池充放电过程中存储颗粒应力产生的影响参数，并推导出存储颗粒材料断裂的可能性。目的是评估多孔电极的微结构设计，以提供快速充放电，但避免造成限制电池性能和可靠性的断裂等机械损伤的可能性。

关键词：锂离子；电池；应力；存储颗粒