Effect of Intercalation Diffusivity When Simulating Mixed Electrode Materials in Li-Ion Batteries

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Abstract

When building physics-based battery models, the amount of needed parameters is one of the most important issues. Some parameters are easily measured while others are not. Studying the published literature it can be observed that researchers reach different results when measuring the same parameter. This is a tedious problem and needs to be taken into account when building physics-based models. One of these parameters is the intercalation diffusion coefficient. Several researchers have presented different results and also a dependency of the lithium concentration in the materials[1][2]. In this contribution, the impact of the diffusion coefficient when simulating mixed electrode materials have been investigated using COMSOL Multiphysics® software. The model is in 1D with graphite anode and a mixture of NMC and LMO as cathode. The electrolyte is 1:2 EC:DMC with 1M LiPF6 . All materials are taken form the material library in COMSOL. The result shows that when the transport in the electrode material is the limiting factor, the diffusion coefficient strongly affects the shape of the simulated potential curve of the battery. This particular issue has only been observed when simulating mixed electrode material. Further it is known that the diffusion coefficient strongly affects the relaxation behavior of the battery. The concentration in the materials holds a high dependency on the diffusion coefficients. As there is a buildup of surface concentration with slow transport of lithium into the particle the relaxation of the battery will also be slower.

Reference

[1] P. C. Goonetilleke et al., Effects of Surface-Film Formation on the Electrochemical Characteristics of LiMn2O4 Cathodes of Lithium Ion Batteries, Journal of the Electrochemical Society, Vol. 156, pp. A709-A719 (2009).

[2] S. L. Wu et al., High Rate Capability of Li(Ni1/3Mn1/3Co1/3)O2 Electrode for Li-Ion Batteries, Journal of The Electrochemical Society, Vol. 159, pp. A438-A444 (2012).

Figures used in the abstract

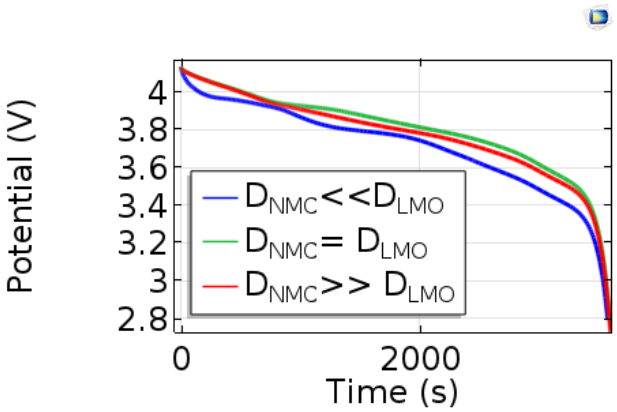

Figure 1: Potential curve when varying the intercalation diffusion coefficients of the cathode materials.

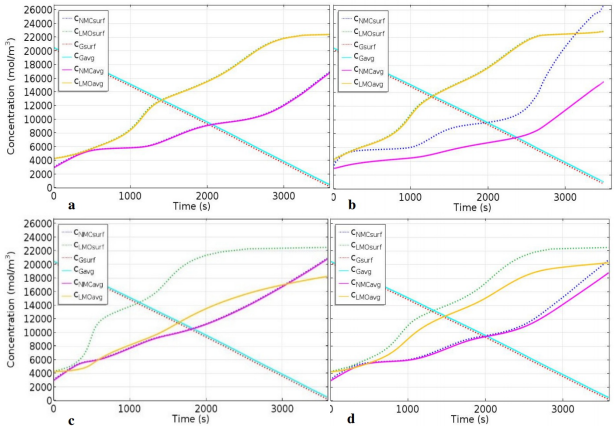

Figure 2: Average lithium concentrations in the cathode materials for the different intercalation diffusion coefficients.