Multiscale Modeling of Magnetic Susceptibility of a LiFePO$_4$ battery

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A major problem in battery management systems (BMS) is the determination of the state of charge (SOC) of the battery [1]. On the one hand, the SOC is important information for the user in order to estimate the remaining working time of the device, i.e. it is an important psychological factor, e.g. in the context of range anxiety in electric vehicles. On the other hand, the knowledge of the SOC is important for the management of the battery since many systems are sensitive to deep discharge or overcharge. These states of extremely high or too low SOC can lead to irreversible damage in the battery [2].

Current strategies for determining the SOC all suffer drawbacks [1]: discharge tests are not online applicable; Coulomb counting needs continuous re-calibration and is sensitive to side reactions; measurement of OCV or EMF need long rest times before they can be applied; impedance spectroscopy is cost intensive and temperature sensitive; artificial neural networks need intensive training with a similar battery; Kalman filters need large computing capacities, a suitable battery model and determination of initial parameters. Therefore, a reliable method for the direct measurement of SOC is desirable.

The idea of this work is to use the change of the paramagnetic properties of the lithium during charge and discharge to determine the SOC. In the literature, numerous examples of the application of nuclear magnetic resonance (NMR) spectroscopy, a similar and related method, for the measurement of lithium ion batteries can be found.

In order to establish a relationship between magnetic susceptibility and SOC a multiscale susceptibility model was coupled with an electrochemical model.
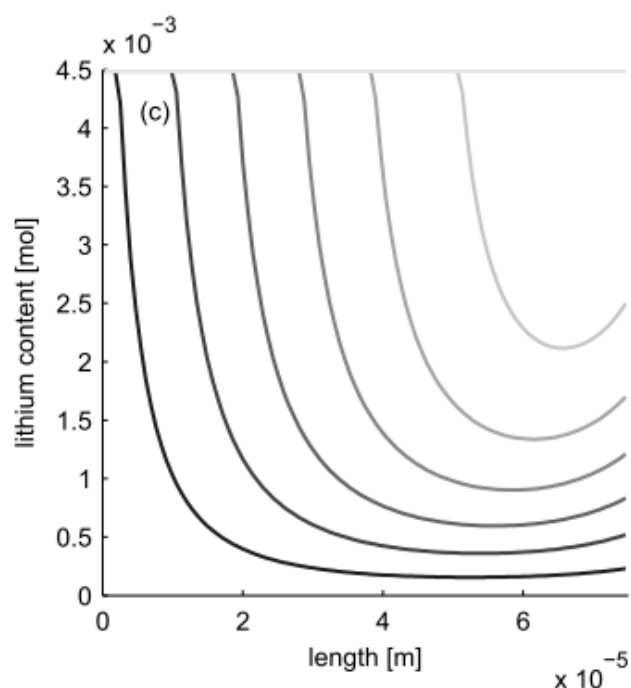
The multiscale susceptibility model describes the relationship between magnetic susceptibility and structure (e.g. porosity, particle size, Li distribution) of a LiFePO$_4$ battery. The electrochemical model describes the structure (especially the Li distribution) as a function of SOC.

The multiscale susceptibility model consists of a molecular level model to describe the susceptibility of Li$_x$FePO$_4$ for various lithium content x. This relation is used in the particle scale of the model to describe the susceptibility of a single electrode particle. At the negative electrode the intercalation of Li into graphite particles is described. At the positive electrode, a phase separation between a Li-rich phase and a Li-depleted phase occurs [3] which is modeled with a core-shell approach.

On the electrode scale of the model, the susceptibilities of the single particles are combined to describe the effective susceptibility of the whole electrode as a function of Li distribution. The Li distribution is determined by an electrochemical model of the battery as a function of SOC, as can be seen in Fig 1.

The electrochemical model uses an established framework of Newman et al. [3] with an additional simplified shrinking-core model of the particles of the positive electrode.

This core-shell structure leads to an interesting hysteresis effect. If the electrode is charged from a fully discharged state, the Li-enriched particles are depleted from lithium. Thus, they have a Li-rich core with a Li-depleted shell surrounding them. If a fully charged electrode is discharged, the Li-depleted particles are enriched with a Li-rich shell, i.e. the phases of the core-shell structure are reversed. This behavior leads to a hysteresis in the magnetic susceptibility as function of SOC, as seen in Fig. 2.

Figure 1: Lithium distribution in the positive electrode as function of state-of-charge.
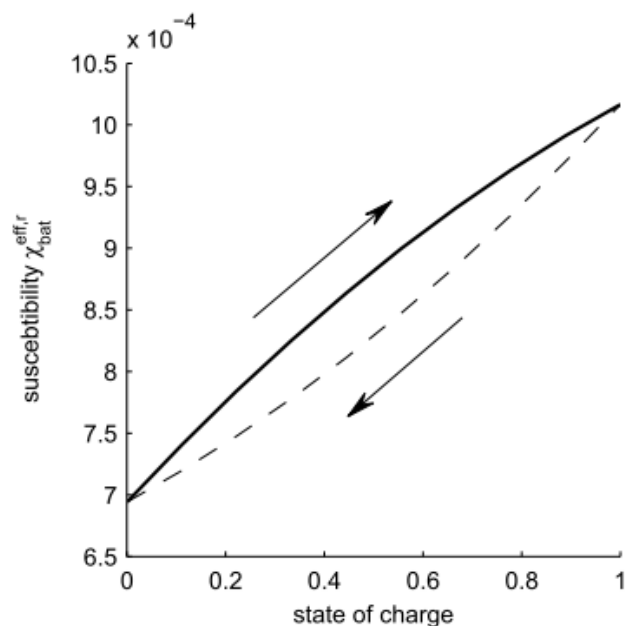
Figure 2: Magnetic susceptibility of a LiFePO4 battery as function of state-of-charge.

[1] V. Pop et al. Meas Sci Tech 2005, 16:R93–R110
[2] K. E. Thomas, R. M. Darling, and J. Newman, Advances in Lithium-Ion Batteries, p. 345, Kluwer Academic/Plenum Publishers, New York 2002
[3] J. Vetter et al. J Power Sources 2005, 147:269–281