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State Estimation of Lithium-Ion Batteries in Aerospace

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Abstract

Lithium-ion batteries are the technology of choice for a broad range of applications due to their performance and long-term stability. The performance and durability of lithium-ion batteries is heavily impacted by various degradation mechanisms. These include the growth of the solid-electrolyte interphase (SEI) and the deposition of metallic lithium on the surface of the negative electrode, also referred to as lithium plating. By comparing electrochemical simulations with experimental measurements, we now perform state-estimation of lithium-ion batteries in order to improve the characterization and management of the battery, e.g., for the battery of the REIMEI satellite. Our goal is to understand the degradation processes and to observe and detect them while the battery is in operation. As a result, this will improve safety and prolong battery life by reducing capacity fade.

Keywords: lithium-ion battery, degradation, 1D+1D model, parameterization

Nomenclature

c	Li-ion concentration
D	diffusion coefficient
$\vec{j}$	electrical current
k	reaction rate constant
$\dot{s}$	sources in phase x
t_+	transference number
U_0	open circuit potential
ϵ	porosity
κ	ionic conductivity
μ	chemical potential
φ_e	electrochemical potential
Φ_s	electrical potential
τ	tortuosity

Abbreviations

SEI	Solid-electrolyte interphase
SOC	State of charge
SOH	State of health

1. Introduction

Lithium-ion batteries are used in various applications like smartphones, laptops, electric vehicles, and satellites. Despite decades of development, they suffer from severe degradation limiting their applicability in astronautics. Long-term SEI growth is the biggest contributor to capacity fade in lithium-ion batteries. Lithium plating, which occurs at low temperatures or high-current charging, can result in capacity fade or even thermal runaway. Our group develops models for SEI growth [1–3]. Furthermore, we simulate lithium plating in the 3D microstructure of a battery [4].

Operando measurement of these meso-scale degradation processes would ensure safe operation of batteries. One summarizes the hidden state of battery degradation with the state-of-charge (SOC) and the state-of-health (SOH). The accurate determination of these states of the battery is a challenging task.

For this purpose, we apply an electrochemical model. The model consists of the pseudo two-dimensional (P2D) approach introduced by Newman et al. [5] and improved by the thermodynamic consistent theory described by Latz and Zausch [6,7].

In this work we compare simulations of the charge and discharge process to experiments with lithium-ion batteries of the satellite REIMEI. The batteries consist of commercial 3Ah $Li_xMn_2O_4$ pouch cells. The satellite REIMEI is a small scientific LEO satellite designed for aurora observations and demonstration of advanced satellite technologies [8,9]. It was designed by the Japan Aerospace Exploration Agency (JAXA).

2. Theory and model

Our model is based on volume-averaged transport theory and Butler-Volmer reaction kinetics [10]. The main dimension of the model describes the transport of ions through the porous cell; an additional dimension takes into account the diffusive transport of lithium inside solid electrode particles and SEI growth. These two dimensions are connected by electrochemical reactions at the electrode-electrolyte interface.

2.1 Transport equations

The transport of lithium ions in an electro-neutral electrolyte is described by continuity equations for lithium ions

$$\partial_t \epsilon_e c_e = \vec{\nabla}\cdot\left(\frac{\epsilon_e}{\tau_e} D_e \vec{\nabla} c_e\right) - \vec{\nabla}\cdot\left(\frac{t_+}{z_+F}\vec{j}_e\right) + \dot{s}_e \qquad (1)$$

and charges

$$0 = \vec{\nabla}\cdot\vec{j}_e + \dot{s}_e \qquad (2)$$

$$= -\vec{\nabla}\cdot\left(\frac{\epsilon_e}{\tau_e}\kappa\,\vec{\nabla}\varphi_e\right) - \vec{\nabla}\cdot\left(\frac{\epsilon_e}{\tau_e}\kappa\,\frac{1-t_+}{z_+\mathrm{F}}\left(\frac{\partial\mu}{\partial c}\right)\vec{\nabla} c_e\right) + \dot{s}_e.$$

The diffusive transport of lithium atoms inside electrode particles is described by

$$\partial_t c_s = \vec{\nabla}\cdot\left(\frac{\epsilon_s}{\tau_s} D_s \vec{\nabla} c_s\right) + \dot{s}_e. \qquad (3)$$

3. Parametrisation

We determine material parameters for an accurate model representation of the battery. To this aim, we adjust the model to the REIMEI battery by comparing our simulations with published half-cell experiments [11]. Important material properties are the cell geometry, electrode structure, transport coefficients, and reaction kinetics.

Subsequently, the parameters for the full cell, in particular the initial SOC before cycling, are determined by comparing simulations with full-cell experiments.

3.1 Experiments

The considered full-cell experiments were performed under the following cycling conditions [9]:

- Slow cycling: C/10 constant current discharge to the lower voltage limit of 3 V followed by C/10 constant current/constant voltage charge to the upper voltage limit of 4.1 V.
- Fast cycling: C/3 discharge and C/2 charge with the cycling conditions of slow cycling.

4. Results

With the obtained parameters the charge and discharge process can be adequately simulated.

4.1 Simulation

The simulations were performed under the same operating conditions as the slow and fast cycling of the full-cell experiments. The comparison of experiment and simulation is shown in Fig. 1. Furthermore, our model simulates the battery state-of-health.

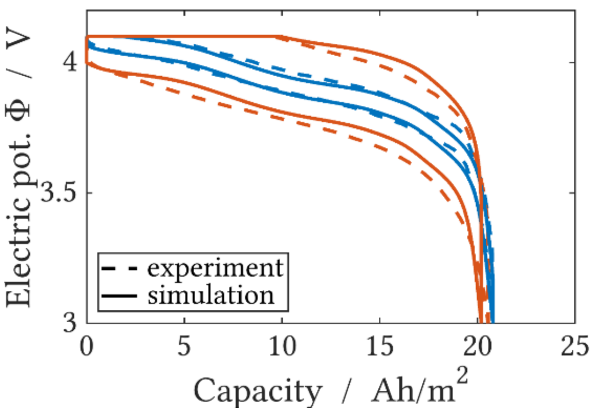

Fig. 1. Simulation and experiment of slow (blue) and fast (red) charge and discharge

5. Conclusion

Fast and slow cycling of a lithium-ion battery were simulated and compared to experiments. In future work, we will incorporate in-flight data of the satellite and sophisticated methods for state estimation to describe the battery degradation.

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References

[1] F. Single, B. Horstmann, A. Latz, Dynamics and morphology of solid electrolyte interphase (SEI), Phys. Chem. Chem. Phys. 18 (2016) 17810–17814.

[2] F. Single, B. Horstmann, A. Latz, Revealing SEI Morphology: In-Depth Analysis of a Modeling Approach, J. Electrochem. Soc. 164 (2017) E3132–E3145.

[3] F. Single, A. Latz, B. Horstmann, Identifying the Mechanism of Continued Growth of the Solid-Electrolyte Interphase, ChemSusChem. 11 (2018) 1950–1955.

[4] S. Hein, A. Latz, Influence of local lithium metal deposition in 3D microstructures on local and global behavior of Lithium-ion batteries, Electrochim. Acta. 201 (2016) 354–365.

[5] M. Doyle, T.F. Fuller, J. Newman, Modeling of

Galvanostatic Charge and Discharge of the Lithium / Polymer / Insertion Cell, J. Electrochem. Soc. 140 (1993) 1526.

[6] A. Latz, J. Zausch, Thermodynamic consistent transport theory of Li-ion batteries, J. Power Sources. 195 (2011) 3296–3302.

[7] A. Latz, J. Zausch, Multiscale modeling of lithium ion batteries: thermal aspects, Beilstein J. Nanotechnol. 6 (2015) 987–1007.

[8] M. Uno, K. Ogawa, Y. Takeda, Y. Sone, K. Tanaka, M. Mita, H. Saito, Development and on-orbit operation of lithium-ion pouch battery for small scientific satellite REIMEI, J. Power Sources. 196 (2011) 8755–8763.

[9] S. Brown, K. Ogawa, Y. Kumeuchi, S. Enomoto, M. Uno, H. Saito, Y. Sone, D. Abraham, G. Lindbergh, Cycle life evaluation of 3 Ah LixMn2O4-based lithium-ion secondary cells for low-earth-orbit satellites. I. Full cell results, J. Power Sources. 185 (2008) 1444–1453.

[10] J. Stamm, A. Varzi, A. Latz, B. Horstmann, Modeling nucleation and growth of zinc oxide during discharge of primary zinc-air batteries, J. Power Sources. 360 (2017) 136–149.

[11] S. Brown, K. Ogawa, Y. Kumeuchi, S. Enomoto, M. Uno, H. Saito, Y. Sone, D.P. Abraham, G. Lindbergh, Cycle life evaluation of 3Ah LixMn2O4-based lithium-ion secondary cells for low-earth-orbit satellites II. Harvested electrode examination, J. Power Sources. 185 (2008) 1454–1464.