Numerical Analysis of a $LiFePO_4$/Graphite Lithium-ion Coin-cell Battery

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Introduction: Lithium-ion batteries (LIBs), based on the $LiFePO_4$/graphite chemistry, attracts nowadays much attention for application in electric vehicles due to the excellent cycling stability of the $LiFePO_4$ electrode. In this work, we present a simulation research based on a two-dimensional axisymmetric model of $LiFePO_4$ (LFP)/graphite lithium-ion batteries using COMSOL Multiphysics@. The spatial distributions of lithium ion concentration, potential and lithium concentration at the electrode particles are obtained. The electrode reaction, discharge characteristics, and the effect of electrode configuration are analyzed.

Computational Methods: The LFP and graphite electrodes with 200 μm thickness used in this study are assembled and sealed in a CR2032-type coin cell. The positive and negative electrodes are separated by a polypropylene separator with 200 μm thickness. The two stainless steel spacers are used between the electrodes and coin cell case and a gasket is used to seal the coin cell. The electrolyte is a liquid electrolyte composed of 1.2 M $LiPF_6$ in 3:7 EC/ EMC solution. The main electrochemical reactions of $LiFePO_4$/graphite LIBs can be represented by

$$\mathrm{C_6} + x\mathrm{Li^+} + xe^- \leftrightarrow \mathrm{Li}_x\mathrm{C_6} \quad (1)$$

$$\mathrm{Li}_{1-x}\mathrm{FePO_4} + x\mathrm{Li^+} + xe^- \leftrightarrow \mathrm{LiFePO_4} \quad (2)$$

The electrochemical reactions are described by a Butler-Volmer expression

$$i_{\mathrm{loc}} = i_0\left[\exp\left(\frac{\alpha_a F\eta}{RT}\right) - \exp\left(\frac{-\alpha_c F\eta}{RT}\right)\right] \quad (3)$$

$$i_0 = F(k_c)^{\alpha_a}(k_a)^{\alpha_c}(c_{s,\max} - c_s)^{\alpha_a}(c_s)^{\alpha_c}\left(c_l/c_{l,\mathrm{ref}}\right)^{\alpha_a} \quad (4)$$

where c_s denotes the concentration of lithium ($\mathrm{Li}\Theta_s$) in the electrode particles, $c_{s,\max}$ is the total concentration of reaction sites, and the state-of-charge variable SOC can be defined by $\mathrm{SOC} = c_s/c_{s,\max}$.

Results: The calculations are performed at the discharge rates of 1/2, 2/3, 1 and 3/2 C. The battery is discharged down to 2.5 V from full-charge state. The ODE Events (*ev*) interface of COMSOL Multiphysics is used to control the end of discharge. In order to compare $LiFePO_4$ (LFP) cathode with other cathode materials, the discharge characteristics of $LiCoO_2$ (LCO)/graphite and $LiMn_2O_4$ (LMO)/graphite coin cells are also calculated.

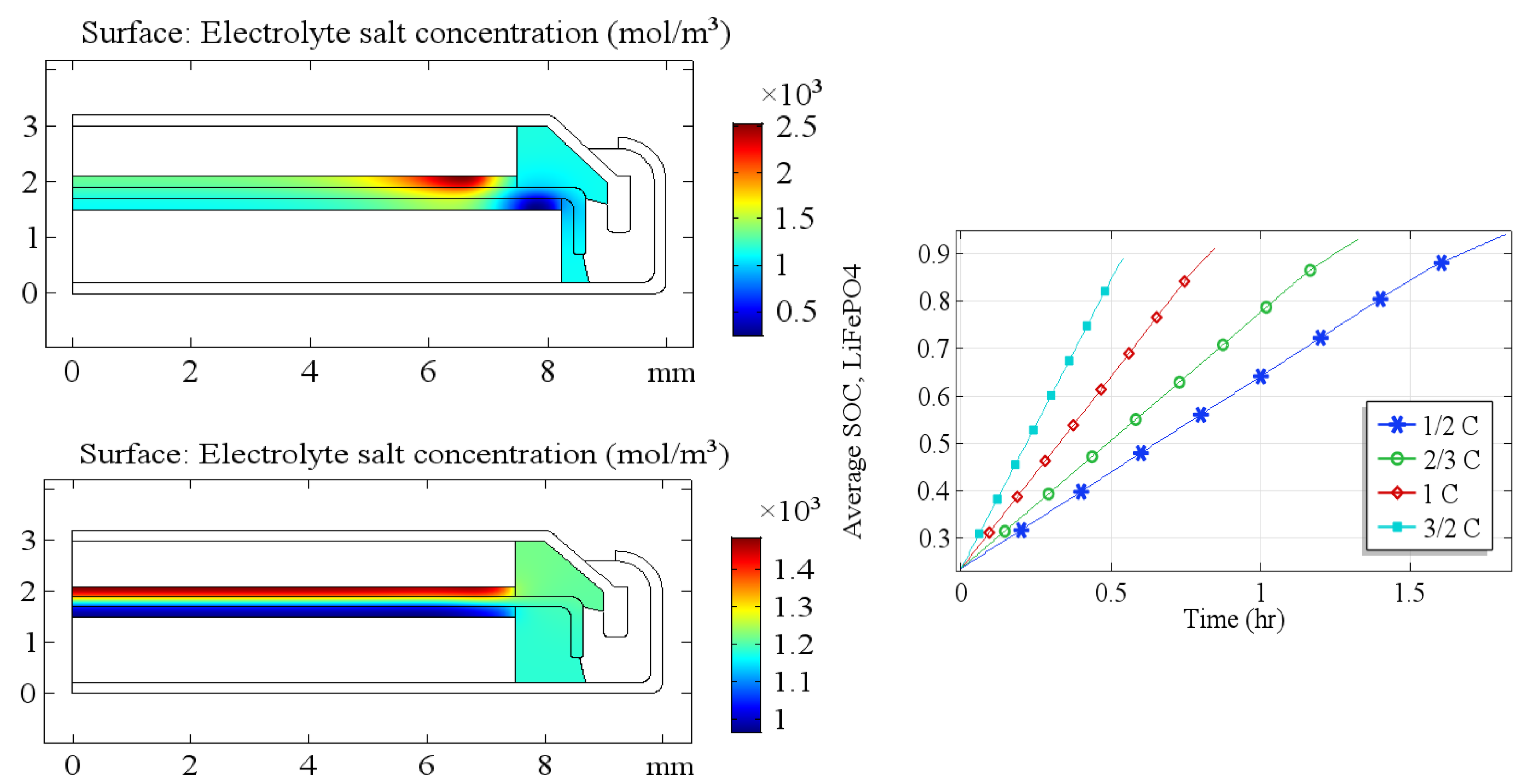

Figure 1. Electrolyte salt concentration at the end of discharge (C-rate=0.5) and average SOC in $LiFePO_4$ during the discharge of a $LiFePO_4$/graphite cell.

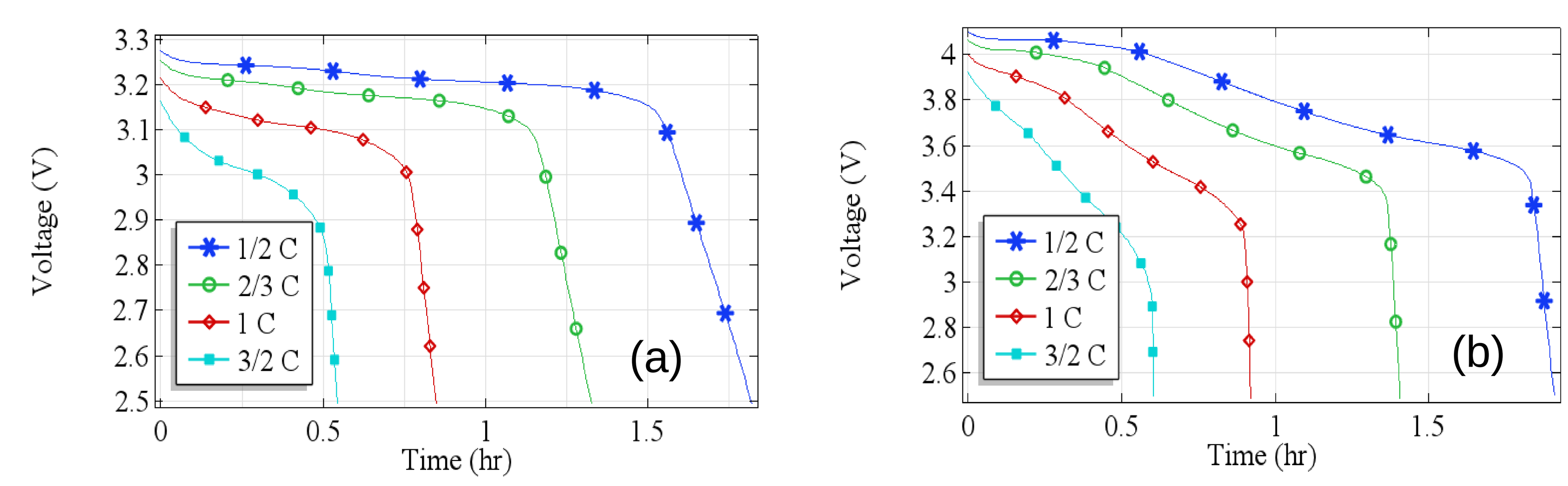

Figure 2. Temporal evolution of cell voltage during the discharge of $LiFePO_4$/graphite(a) and $LiCoO_2$/graphite(b) coin cells.

Since the capacity of LCO cathode is much higher than that of graphite, here we reduce the thickness of LCO to make the capacity of LCO be the same as that of graphite.

Conclusions: This paper reports the simulation results of a $LiFePO_4$/graphite lithium-ion coin cell battery. It is found that the distributions of lithium ion concentration, potential and lithium concentration at the electrode particles can be improved by adjusting the electrode configuration. At low discharge rates, the decrease of the cell voltage of $LiFePO_4$/graphite before depletion is much slower than those of other cathode materials, which would be beneficial in industrial applications of $LiFePO_4$ in near future.

References:

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