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A two-dimensional modeling of a lithium-polymer battery

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Abstract

The potential and current density distribution on the electrodes of a lithium-polymer battery were studied by using the finite element method. The effect of the configuration of the electrodes such as the aspect ratio of the electrodes and the size and placing of current collecting tabs as well as the discharge rates on the battery performance was examined to enhance the uniformity of the utilization of the active material of electrodes. The results showed that the aspect ratio of the electrodes and the size and placing of current collecting tabs have a significant effect on the potential and current density distribution on the electrodes to influence the distribution of the depth of discharge on the electrodes, thus affecting the uniform utilization of the active material of electrodes.

Keywords: Lithium-polymer battery; Model; Electrode configuration; Potential distribution; Current density distribution; Finite element method

1. Introduction

There is a significant interest in the use of batteries for hybrid electric vehicle (HEV) and electric vehicle (EV). The outstanding characteristics of lithium-polymer batteries (high energy density, high voltage, low self-discharge rate, and good stability among others) make them one of the preferred choices for such applications. However, much larger lithium-polymer batteries than those available in the market for consumer electronics are required for HEV and EV applications. The performance of a battery electrode is influenced by the aspect ratio, the placing of current collecting tabs, and the total amount of the current flowing through an electrode. If an electrode is not designed optimally, the potential and current density will be non-uniformly distributed, and the utilization of the active material over the electrode will be non-uniform. Accelerated degradation of the electrode may result due to excessive localized utilization of the active material on the electrode. That effect becomes more pronounced, as the size of the electrode becomes larger. Therefore, an optimum design of the electrode is pertinent for the production of large-scale lithium-polymer batteries.

When scaling up a small-scale cell to a large-scale battery, mathematical modeling plays an important role, because nearly limitless design iterations can be performed by using simulations [1]. Previous reviews of the modeling of lithium batteries are given in references [2–5]. A one-dimensional model assumes that the gradients of the variables adopted in modeling are negligible in the two directions parallel to the current collectors. Such an assumption may be valid for small-scale cells. However, that assumption may not be justified for large-scale batteries, since the potential drop along the current collector due to ohmic drop may be significant enough to affect the current distribution, with a higher current closer to the tabs. Then, a two- or three-dimensional model may be desirable for large-scale batteries [6–9].

In this work, a two-dimensional modeling is performed to calculate the potential and current density distribution on the electrodes of a lithium-polymer battery comprising a $LiMn_2O_4$ cathode, a graphite anode, and a plasticized electrolyte. This work adopts a relatively simpler modeling approach by considering only Ohm's law and charge conservation on the electrodes based on the simplified polarization characteristics of the electrodes as compared to the previously published papers by other researchers [10–15]. The distribution of the depth of discharge (DOD) on the electrode is predicted as a function of discharge time from the calculated potential and current density distribution. Based on the distribution of DOD, the effects of the aspect

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ratio of the electrodes, the size and placing of current collecting tabs, and discharge rates on the battery performance are evaluated.

2. Mathematical model

A schematic diagram of the current flow in the parallel plate electrodes of a battery is shown in Fig. 1. The distance between the electrodes is assumed to be so small that the current flow between the electrodes is perpendicular to the electrodes. From the continuity of current on the electrodes, the following equations can be derived:

$$\nabla \cdot \vec{i}_p - J = 0 \quad \text{in} \ \Omega_p \tag{1}$$

$$\nabla \cdot \vec{i}_n + J = 0 \quad \text{in} \ \Omega_n \tag{2}$$

where $\vec{i}_p$ and $\vec{i}_n$ are the linear current density vectors (current per unit length (A cm^{-1})) in the positive and negative electrodes, respectively, and J is the current density (current per unit area (A cm^{-2})) transferred through the separator from the negative electrode to the positive electrode. Ω_p and Ω_n denote the domains of the positive and negative electrodes, respectively. By Ohm's law, $\vec{i}_p$ and $\vec{i}_n$ can be written as

$$\vec{i}_p = -\frac{1}{r_p}\nabla V_p \quad \text{in} \ \Omega_p \tag{3}$$

$$\vec{i}_n = -\frac{1}{r_n}\nabla V_n \quad \text{in} \ \Omega_n \tag{4}$$

where r_p and r_n are the resistances (Ω) of the positive and negative electrodes, respectively, and V_p and V_n are the potentials (V) of the positive and negative electrodes, respectively. By substituting Eqs. (3) and (4) into Eqs. (1) and (2), the following Poisson equations for V_p and V_n are obtained:

$$\nabla^2 V_p = -r_p J \quad \text{in} \ \Omega_p \tag{5}$$

$$\nabla^2 V_n = +r_n J \quad \text{in} \ \Omega_n \tag{6}$$

The relevant boundary conditions for V_p are

$$\frac{\partial V_p}{\partial n} = 0 \quad \text{on} \ \Gamma_{p_1} \tag{7}$$

$$-\frac{1}{r_p}\frac{\partial V_p}{\partial n} = \frac{I_0}{L} \quad \text{on} \ \Gamma_{p_2} \tag{8}$$

where $\partial/\partial n$ denotes the gradient in the direction of the outward normal to the boundary. The first boundary condition (7) implies that there is no current flow through the boundary (Γ_{p_1}) of the electrode other than the tab. The second boundary condition (8) means that the linear current density through the tab (Γ_{p_2}) of the length L (cm) is constant to the value of I_0/L. I_0 is the total current (A) through the tab in the mode of constant-current discharge. The boundary conditions for V_n are

$$\frac{\partial V_n}{\partial n} = 0 \quad \text{on} \ \Gamma_{n_1} \tag{9}$$

$$V_n = 0 \quad \text{on} \ \Gamma_{n_2} \tag{10}$$

The first boundary condition (9) implies the same as in the case of V_p. The second boundary condition (10) means that the potential at the tab of the negative electrode is fixed to the value of zero as the reference potential.

The resistance, r (r_p or r_n), is calculated as follows:

$$r = \frac{1}{h_c S_c + h_e S_e} \tag{11}$$

where h_c and h_e are the thicknesses (cm) of the current collector and the electrode material, respectively, and S_c and S_e are the electrical conductivities (S cm^{-1}) of the current collector and the electrode material, respectively. The parameters used in the calculations of resistances for the electrodes are listed in Table 1. The values of electrical conductivities of composite electrodes are the same as those used in the references [14,15]. The current collectors of cathode and anode are made of aluminum and copper, respectively.

The current density, J, of Eqs. (5) and (6) is the function of the potential difference between the positive and negative electrodes, ($V_p - V_n$). The functional form depends on the polarization characteristics of the electrodes. In this study, the following

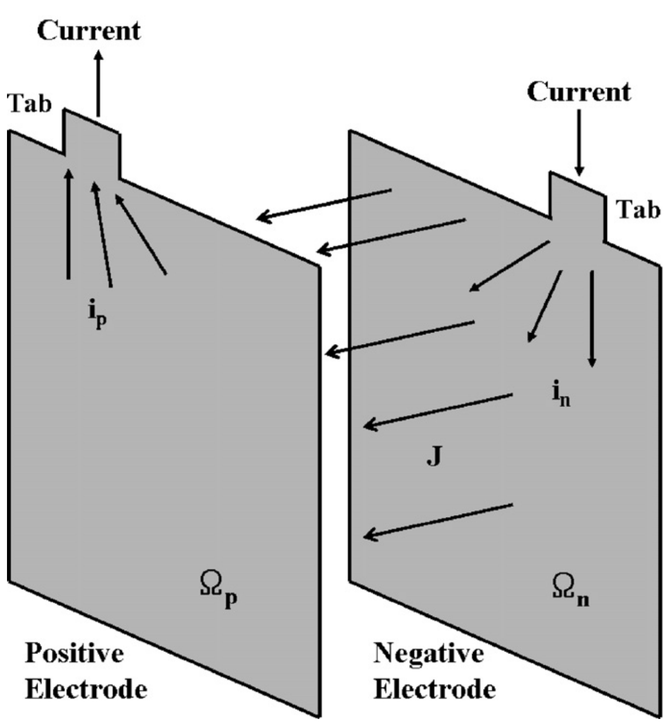

Fig. 1. Schematic diagram of the current flow in the parallel plate electrodes of a battery.

Table 1
Parameters for the electrodes

Parameter	Li_xC_6	$Li_yMn_2O_4$
S_e (S cm^{-1})	1.0	0.038
h_e (μm)	85	140
S_c (S cm^{-1})	6.33×10^5	3.83×10^5
h_c (μm)	10	20