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Lattice Boltzmann simulation of ion and electron transport in lithium ion battery porous electrode during discharge process

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Abstract

A two dimensional lattice Boltzmann simulation of ion and electron transport within lithium ion battery porous electrode was presented in this study. In the simulation, a LiyC6|LixMn2O4 rocking-chair rechargeable battery structure was employed and the electrode was composed of irregular particles. The effects of electrode micro-structure on the local lithium concentration distribution, electric potential and macroscopic discharge performance were investigated. Results show that smaller particles were lithiated and delithiated at a higher rate during the discharge process. The lithium depletion in anode and the lithium accumulation in cathode were enhanced in the edges and corners for large irregular particles. The particles with lower lithium concentration produced higher local electric potential in the anode. For discharge performance, the porosity of the electrode had significant influence on the achievable capacity.

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Keywords: Lithium ion battery; Electrode micro-structure; Lattice Boltzmann method; Discharge process

1. Introduction

In the last two decades, Lithium ion battery (LIB) has become one of the most important power sources for portable devices, electric vehicles and power grid. Due to the increasing demand for environmentally friendly and fuel economy vehicles, automotive companies are paying a lot of effort on electric vehicles and hybrid electric vehicles (HEVs). These vehicles would enable meeting the demands

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for electrical power due to the increasing use of the electronic features to improve vehicle performance, fuel economy, emissions, passenger comfort, and safety. As a result, it is important to have a firm understanding of working process and conductive mechanisms in LIB. Many experimental studies have reported linkages between morphology of constituent electrode and battery performance [1-3]. Investigations on the effect of electrode with 2D or 3D micro-structure were reported in literature [4-6]. LBM is a good approach to solve the diffusion-reaction problems within complex geometry [7, 8]. In this study, we develop a two dimensional framework for LBM simulation of ion and electron transport in the LIB porous electrode. A $Li_yC_6|Li_xMn_2O_4$ rocking-chair rechargeable battery structure is employed in our study. The battery electrode is comprised of active cathode and anode particles and electrode with different particle shape and porosity is considered. The effects of the electrode micro-structure on lithium concentration and electric potential distribution and the battery performance are investigated.

2. Theory and Modeling

2.1. Theoretical model

In the electrolyte phase, the transport of lithium ion and electron are given by a set of partial difference equations which derive from a Nernst-Plank model.

$$\nabla \cdot \kappa \nabla \phi + \nabla \cdot \left(\frac{D_{Li} z F C_{Li}}{RT} \nabla C_{Li} \right) = 0 \tag{1}$$

$$\frac{\partial C_{Li}}{\partial t} - \nabla \cdot \left(D_{Li} \nabla C_{Li} \right) - \nabla \cdot \left(\frac{D_{Li} z F C_{Li}}{RT} \nabla \phi \right) = 0 \tag{2}$$

where ϕ is the electric potential, κ is the electrical conductivity. C_{Li} is the lithium ion concentration, D_{Li} is the diffusivity of lithium ion. Within the electrode particles, Eq. (1) and Eq. (2) can be reduced to classic diffusion and charge continuity equation by setting z=0.

2.2. Lattice Boltzmann method

LBM is utilized to solve the governing equations of the transport of ion and electron. Within the electrolyte phase, the following evolution equations are used to describe the ion transport and the electron conduction [9].

$$g_{i,k}\left(\mathbf{x}+\mathbf{c}_i\Delta t, t+\Delta t\right) - g_{i,k}\left(\mathbf{x},t\right) = -\frac{1}{\tau_{D,k}}\left(g_{i,k}\left(\mathbf{x},t\right) - g_{i,k}^{eq}\left(\mathbf{x},t\right)\right) + \frac{zF\left(\mathbf{c}_i-\mathbf{u}\right)\cdot\nabla\phi}{RT} g_{i,k}^{eq}\left(\mathbf{x},t\right) \tag{3}$$

$$h_i\left(\mathbf{x}+\mathbf{c}_i\Delta t, t+\Delta t\right) - h_i\left(\mathbf{x},t\right) = -\frac{1}{\tau_h}\left(h_i\left(\mathbf{x},t\right) - h_i^{eq}\left(\mathbf{x},t\right)\right) + \omega_i \frac{F\nabla\cdot\left(zD\nabla C_{Li}\right)}{RT} \tag{4}$$

where $g_{i,k}$ and h_i are the distribution functions of specie concentration and electric potential, $g_{i,k}^{eq}$ and h_i^{eq} are the corresponding equilibrium functions, respectively. Within the electrode particles, Eq. (3) and Eq. (4) can be reduced to classic evolution equations by setting z=0.

3. Results and discussion

From the LBM calculation, the microscopic distribution of lithium ion and electric potential in the electrode and the macroscopic cell voltage can be obtained. Simulation results of Fig.1 show the time evolutions of the lithium concentration in the battery electrode with irregular geometry. As depicted in