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Improving wettability and preventing Li-ion batteries from thermal runaway using microchannels

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ABSTRACT

Effects of using microchannels on the wettability of the porous electrodes and preventing the battery cell from thermal runaway have been studied. Two-dimensional Lattice Boltzmann Method (LBM) simulation was carried out to simulate the effects of embedded microchannels inside the electrodes on the electrolyte transport in the porous electrodes as well as their effects to lead the generated gases during thermal runaway out of the battery cell. The two-phase intermolecular potential model was utilized to investigate the microscopic behavior of the electrolyte flow in the porous electrodes. The results showed that embedding microchannels inside the electrodes significantly improves the wettability of the electrodes, especially for the electrodes with lower porosities. Furthermore, the use of microchannels inside the electrodes could considerably reduce possibility of occurrence of the thermal runaway. During thermal runaway, the electrodes with higher number of smaller microchannels could drive the generated gases out of the battery cell much quicker than the electrodes with lower number of larger microchannels.

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1. Introduction

High power Li-ion batteries are the targets of recent studies for electric and hybrid electric vehicles industry. Based on the United States Advanced Battery Consortium (USABC), the long term goals for energy and power densities are 300 Wh/L and 600 W/L, respectively [1]. To meet these goals, it is necessary to make Li-ion batteries with highly compressed electrodes. Higher compression causes lower porosity and increases the pore blockage. The pore blockage decreases the wettability of the electrodes and leads to lower performance of the batteries. Therefore, one of the critical factors that effects on the performance and lifespan of the Li-ion batteries is the wettability of the electrodes.

To maintain high utilization of electrode capacity, the electrode should be fully wetted with the electrolyte. If an electrode is insufficiently wetted, electrolyte resistance increases and the use of electrode capacity would be poor and insignificant. The battery performance would be deteriorated by insufficient wetting. Furthermore, this phenomenon leads to extrusion of lithium metal that decreases the safety of the battery. Moreover, the degradation of Li-ion batteries would be accelerated by insufficient wetting that decreases the life of the batteries [2].

Therefore, understanding the microscopic behavior of the electrolyte flow in the separator and electrodes is necessary and inevitable. In this regard, the effects of surface free energy and contact angle on various separators and electrodes were investigated by Stefan et al. [3] at a series of room temperatures. Their results showed that separator wettability is one of the most important parameters that should be considered in electrochemical devices. Xie et al. [4] showed that good wettability of the polyolefin separator had positive impacts on the lithium dendrite suppression and rate performance of lithium metal batteries. Liu et al. [5] introduced a new separator using surface chemical modification and showed that their modified separator had better wettability and thermal stability.

Natural graphite was examined by Menachem et al. [6], and better performance was obtained from better wetting of the electrolyte. The wettability of both the anode and cathode was studied experimentally by Wu et al. [7]. Their results showed that wettability of the porous electrodes is controlled mainly by electrolyte penetration and spreading in pores. Also, organic solvent composition and lithium salt concentration effect on the wettability of the electrodes, by changing the viscosity and surface tension of the electrolyte. Yu et al. [8] showed that at high current rates, insufficient wetting of the thick and dense electrodes degrade discharge capacity rapidly. The influence of compaction on the porosity and electrochemical properties of a positive electrode was studied by

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Nomenclature

Ca	capillary number
c_s	speed of sound (m/s)
e_i	lattice velocity (m/s)
f	distribution function
F_γ	*Shan Chen force*
G	Green's function (simple scalar)
p	pressure (pas)
Δp	pressure difference (pas)
r	radius of the droplet (m)
Re	Reynolds number
S	source term
u	velocity (m/s)
w	weight coefficient

Greek

ρ	density (kg/m^3)
υ	kinetic viscosity (m^2/s)
σ	surface tension (N/m)
ψ	function of density
τ	relaxation time
μ	dynamic viscosity (kg/m s)

Subscript

eq	equilibrium
γ	component
in	inside
out	outside

Chu et al. [9]. Their results showed that at high C rates, wettability would be predominant.

Recently, Lattice Boltzmann Method (LBM) has been utilized to simulate multi-phase and multi-component fluid flows. This method is based on the mesoscopic kinetic theory of the fluids, and because of its ability to study complex boundaries, it has become a promising computational method for simulating various fluid applications such as porous media. Therefore, LBM is an appropriate approach to simulate electrolyte transport in a porous electrode. Lee et al. [2] numerically investigated the electrolyte transport in the porous electrode using the two-dimensional LBM. Dynamic behavior of the liquid electrolyte and wettability of the electrode were studied, and it was shown that the wettability is affected strongly by two-phase (electrolyte and air) transport. They also showed that LBM could be effectively carried out to simulate liquid electrolyte behavior in the porous electrodes. In another study, Lee and Jeon [1] investigated the wettability of the porous electrodes paying attention to the compression ratio of the electrodes and found wettability reduction by increasing the compression ratio. Their results also showed that due to the deformation of particle shape, negative electrode had lower wettability than the positive one.

In the past decade, thermal management improvement of Li-ion batteries, and preventing them from thermal runway have been the concerns of high power demand industries. Many studies have been done using different kind of external cooling methods such as pin fin heat sinks [10,11], phase change materials [12,13], porous metal foams [14,15], mini- and microchannels [16,17], and heat pipes [18,19]. Among these studies, some researchers suggested that some external thermal management systems were not successful to prevent the batteries from thermal runaway. For example, Xu et al. [20] investigated the influence of the minichannels on thermal runaway that was caused by nail penetration. Their results showed that thermal runaway in the battery cell was not preventable using the minichannel cooling system. Therefore, the need to find new thermal management systems is pressing. One of these novelty systems that was proposed by the authors [21,22] was flowing liquid electrolyte through microchannels embedded inside the electrodes for cooling purposes. These microchannels are not only efficient for cooling purposes but can also be used to drive the generated gases out of the battery cell during thermal runaway.

In this study, the liquid electrolyte transport in a porous electrode was studied numerically. A 2-D LBM approach has been carried out and the two-phase intermolecular potential model [23,24] was utilized to investigate the microscopic behavior of the electrolyte flow in the porous electrodes. Since the two main challenges for the wettability of Li-ion batteries are enhancing the wettability of the electrodes and improving the electrolyte filling time [2], the objective of this study is to improve both of the challenges by embedding microchannels inside the electrodes. Furthermore, these microchannels would be the best ways to take the released gases during thermal runaway out of the electrode to prevent the battery from further damages and explosion.

2. Model description

2.1. LBM model

The Lattice Boltzmann Method (LBM) has been originated from lattice gas automata (LGA). This method is derived from the continuous Boltzmann equation numerically and is discretized in time and phase space [25]. Distribution function is utilized in the LBM instead of particle population in the LGA. The simple law of collision and streaming steps calculates the time variation of the distribution functions. In this study, the lattice Bhatnagar-Gross-Krook (BGK) model was implemented to approximate the collision term. The discrete particle distribution functions f_i are:

$$f_i(x + e_i\Delta t, t + \Delta t) = f_i(x,t) - \frac{\Delta t}{\tau}\left[f_i(x,t) - f_i^{eq}(x,t)\right] + S_i(x,t) \tag{1}$$

where $f_i(x,t)$ is the probability of finding a particle in the ith velocity e_i at (x,t), Δt is the time step, $S_i(x,t)$ is a source term, and τ is the dimensionless relaxation time that controls the tendency of the system to relax the local equilibrium, and is related to the kinetic viscosity υ. f_i^{eq} is the equilibrium distribution and is given as follows:

$$f_i^{eq} = \rho w_i\left(1 + \frac{\vec{e_i}.\vec{u}^{eq}}{c_s^2} + \frac{\left(\vec{e_i}.\vec{u}^{eq}\right)^2}{2c_s^4} + \frac{\left(\vec{u}^{eq}\right)^2}{2c_s^2}\right) \tag{2}$$

where c_s is the speed of sound that defines as c/3: $c = \Delta x/\Delta t$, and w_i is the weight factor. As two-dimensional nine velocities (D2Q9) model was utilized in this study, and w_i is defined as follows:

$$w_i = \begin{cases} \frac{4}{9} & i = 1 \\ \frac{1}{9} & i = 2,3,4,5 \\ \frac{1}{36} & i = 6,7,8,9 \end{cases} \tag{3}$$

and the discrete velocity e_i defines as

$$[e_1, e_2, e_3, e_4, e_5, e_6, e_7, e_8, e_9] = \begin{bmatrix} 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & -1 \\ 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \end{bmatrix} \tag{4}$$

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