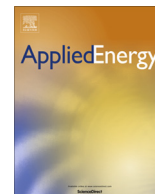




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A microscopic investigation of ion and electron transport in lithium-ion battery porous electrodes using the lattice Boltzmann method

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HIGHLIGHTS

- Lattice Boltzmann method is utilized to predict the ion and electron transport.
- The lithium concentration and electric potential distribution were obtained.
- The particle size and electrode porosity affect the discharge process.
- The electrode microstructure affects the battery performance.

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ABSTRACT

Improving the cycle life and reliability of a battery is an important issue in lithium-ion battery (LIB) applications. Except for the material properties of the battery electrodes, the morphological features of LIBs also have a great influence on battery performance. In order to identify the relation between the morphological features of the electrodes and the macroscopic battery performance, a two-dimensional (2D) lattice Boltzmann model of ion and electron transport within LIB porous electrodes is presented in this study. The proposed model is superior to previous finite element method (FEM)-based models by providing a more convenient geometry generation process and a more efficient calculation technique. In the simulation, the lattice Boltzmann method (LBM) is utilized to solve the governing equations for ion and electron transport. The quartet structure generation set (QSGS) is employed to generate the electrode geometry with circular particles. The effects of the electrode micro-structure on the local concentration distribution, electric potential, and macroscopic discharge performance are investigated. Results show that the LBM is an optional approach in solving problems related to mass transport and electrochemical reactions. For the electrode particles, the obvious variations in local lithium concentration and electric potential prove that the electrode microstructure can influence the microscopic lithium transport; specifically, the lithium exchange is improved for smaller particle sizes. As for discharge performance, larger discharge depth can be achieved by a smaller cathode particle size and a larger cathode porosity. Meanwhile, a larger anode particle size and a smaller anode porosity both contribute to a larger discharge depth.

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1. Introduction

In the last two decades, lithium-ion batteries (LIB) have become one of the most important power sources for portable devices, electric vehicles (EV), power grids, and energy storage devices. Their widespread use can be attributed to their significant advantages, such as long life cycle, large energy density, no memory effect, and environment-friendly features. However, as mentioned in previous investigations [1,2], capacity fading, insufficient power

and energy density, as well as reliability issues still limit the performance of current LIB technologies. Within the limits, the morphological features of electrodes have a significant impact on ion and electron transport. Investigating the electrodes' morphological properties is essential in overcoming the disadvantages in LIB application and improve the battery's cycle life and reliability. Along this line, identifying the relation between microscopic transport mechanisms and macroscopic battery performance is also important.

Generally, LIBs are composed of the cathode material, anode material, and a separator. The electrochemical potential drives the reversible lithium intercalation in the electrode particles, as

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Nomenclature

c	discretized velocity direction	κ	ion conductivity
c_s	lattice sound speed	σ	proton conductivity
C	concentration	τ	relaxation time
D	diffusivity	ω	weight factor
F	Farady constant	y	surface to maximum concentration ration
g	concentration distribution function	ϕ	electric potential
h	potential distribution function		
H	height		
i_0	exchange current density	<i>Superscripts</i>	
I	current density	<i>eq</i>	equilibrium
L	length	<i>neq</i>	non-equilibrium
J	specially chosen constant in Eq. (14)	<i>max</i>	maximum
k	reaction rate in Eq. (6)		
K	specially chosen constant in Eq. (14)	<i>Subscripts</i>	
n	normal vector	<i>a</i>	anode
R	gas constant	<i>c</i>	cathode
t	time	<i>e</i>	electrolyte
t_0	time scale	<i>g</i>	gas
T	temperature	<i>i</i>	direction of the lattice velocity
u	velocity vector	<i>k</i>	kth component
Δx	space step	<i>l</i>	lattice unit
Δt	time step	<i>Li</i>	lithium ion
α	reaction rate coefficient	<i>p</i>	physical unit
η	over-potential	<i>sruf</i>	surface

well as the ion diffusion and migration within the electrolytes passing through the porous electrode architecture. The electrode material and the adhesive composite form a porous structure. Moreover, the macroscopic battery performance is highly related to the microscopic transport within the porous structure. The transport of the lithium ion and electron in the porous electrodes are mainly affected by the material property and electrode morphology. Numerous experimental investigations and numerical simulations have been performed to determine the influence of the transport phenomenon on cell performance. In experimental studies, the morphological features, such as particle shape, particle size, and particle arrays of electrode material, have been found to have a significant influence on cycling performance and battery capacity. For instance, Wu et al. [3] reported that better performance could be achieved when particles have an average size of 200–300 nm and homogeneous distribution for LiMn_2O_4 cathode. Cho and Park [4] concluded that the cathode with a particle size of 13 nm demonstrated a high special capacity. However, obvious limitations in experimental studies also exist, especially because the morphological features of electrode particles, which are produced by chemical and physical preparations, are stochastic and difficult to regulate. Thus, obtaining the exact quantitative relations between morphological features and the macroscopic performance remains a challenge. Furthermore, the uneven local lithium concentration and potential distribution caused by the inhomogeneous morphological features cannot be determined by utilizing existing experimental techniques. As discussed above, experimental investigations cannot sufficiently account for the microscopic transport mechanism. In this case, numerical methods should be employed in investigating the influence of microscopic electrode morphology on the material transport and battery performance.

The development of a numerical method that spatially resolves the electrochemical behavior of an LIB allows us to investigate the transport phenomenon in porous electrodes. The mean-field pseudo two-dimensional (P2D) model, first proposed by Newman et al. [5,6], incorporates a battery's microstructural features into battery models. Instead of using anisotropic material properties,

they used the homogenized spatial distribution of electrode material and electrode porosity to reflect the microscopic effect. The P2D model has been extended by many researchers in subsequent years. In the following investigations, Xie et al. [7] modeled the capacity fading processes, Miranda et al. [8] studied the geometry effect, and Zhao et al. [9] incorporated the thermal effects into the P2D model to predict battery temperature. The abovementioned mean-field continuum models helped improve the battery design in some aspects, but they largely ignore the randomness of electrode particle size, particle shape, and particle distribution. As a result, the influences of electrode microstructure on the performance of LIB have yet to be fully taken into consideration. To describe the impact of the heterogeneity of porous electrode particles on battery performance, generating electrode geometry with anisotropic physical properties and randomly distributed particles is important during the numerical investigation.

To reflect the anisotropic properties of the battery electrode, microscopic investigations are proposed, and different approaches are used to represent the electrode geometry. The regular-shaped and randomly distributed particles are mostly utilized to represent the heterogeneity of electrode particles. For instance, García et al. [10] generated electrodes with randomly distributed circular particles to analyze the effect of microstructure on the power density and chemically induced stresses. Less et al. [11] utilized aggregated cubic particles to form the electrode geometry, and then investigated the effect of packing arrangement and tortuosity on electrode geometry. The utilization of randomly distributed particles has been proven to be superior to mean-field method, because this kind of simulation can reveal microscopic physical processes and identify the local variations of lithium ion and electric potential. In the numerical investigations mentioned above, the finite element method (FEM) is mostly utilized to solve the charge and species transport and understand the battery's electrochemical system. However, difficulties may occur when dealing with the porous electrode geometry. The self-programming code and commercial software are mostly employed to build the geometry and deal with the governing equations. Generally, when large

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