



A computational investigation of thermal effect on lithium dendrite growth

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ABSTRACT

This paper aims to computationally investigate the thermal effect, combining the internal heat and the ambient temperature, on the lithium (Li) dendrite growth process. To achieve this, the recently developed phase-field Li-dendrite model is further extended by coupling with a heat transfer model. The two models are linked via a temperature-dependent ion diffusion coefficient to investigate the evolution of the morphology and size of dendrites. Three levels of cases are used to progressively investigate the thermal effect on Li dendrites: (1) uniform ambient temperature, (2) temperature gradient along the charging direction, and (3) internal heat-induced spatially distributed temperature. The results show that the normalized dendrite length decreases as the ambient temperature increases, which agrees well with the published experimental measurements. The temperature gradient is applied in the 2-D system showing that the formation of lateral branches can be prevented with the presence of the temperature gradient. The third case shows that the temperature significantly increases at the dendrite-electrolyte interface, and the dendrite deviates from the tree-type shape to a nearly rhombic shape. The simulation results provide valuable bases for the future comprehensive studies of the temperature-dependent Li dendrite growth process.

1. Introduction

Lithium (Li) dendrite has been widely observed as batteries undergo cycle-to-cycle charge/discharge processes, and is of great significance to the current and future battery technologies. Li-ion batteries with high energy densities and excellent cycle performance [1–4] are now widely used in the automotive and portable energy storage markets such as electric vehicles [5–7], mobile phones, tablet computers and laptops [8]. Hence, more and more researchers focus on the studies of higher performance Li-ion batteries. However, emerging Li-O₂ (lithium-oxygen) and Li-S (lithium-sulfur) batteries with higher capacities are facing critical issues of Li dendrites on the Li-metal electrodes which significantly hinder the developments and applications of them in industries. Li dendrites formed on the electrode surface during the charging process can damage the battery life, reduce its capacity, and even lead to the battery short-circuit [9]. Therefore, Li dendrite growth mechanisms still represent the subject of numerous research efforts. Several methods have been reported to modulate the dendrite growth such as electrode surfaces roughness [10,11], current densities [12], mechanical forces [13], electrolyte compositions [14], temperature effects [15], interfacial studies [16] and electrode materials [17–20].

Numerous mathematical models have been proposed to reveal the

growth mechanisms of the Li dendrite. For instance, Monroe and Newman [21] established a Li-dendrite growth dynamics model to investigate the effect of the current density and developed a comprehensive theory to elucidate the temporal evolution of the Li-dendrite tip height and the growth velocity. Recently, Akolkar [22,23] proposed an extended model via combining the concentration-dependent diffusion coefficient with the liquid electrolyte to analyze different overpotentials underplay at the electrode surface. Aryanfar et al. [24] presented a Monte-Carlo method to investigate the dendrite growth mechanism with handling the ions migration in electric fields. More recently, Chen et al. [25,26] proposed a nonlinear phase-field model to predict the dendritic patterns during the battery charging with applied voltages and initial electrode morphology conditions, based on the Butler-Volmer kinetics and the thermodynamics. Meanwhile, a phase-field kinetics model was reported by Ely et al. [27] to reveal mechanisms of the local heterogeneous growth and the coarsening of the Li dendrite growth by utilizing an extended asymptotic analysis [28]. Raj and Wolfensine [29] developed an analytical model including the electrochemo-mechanical potential to study the effect of current densities on the dendrite formation. However, these models, to our best knowledge, were limited to a constant room temperature and did not investigate the thermal effect on the Li dendrite growth.

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Nomenclature

a_s	specific surface area per unit volume of the electrode
b	the activation energy (mol m^{-3})
c	concentrations of species (mol m^{-3})
C_{ps}	specific heat capacity in electrolyte ($\text{J kg}^{-1} \text{K}^{-1}$)
C_{pe}	specific heat capacity in electrode ($\text{J kg}^{-1} \text{K}^{-1}$)
D_e	diffusion coefficient in electrode ($\text{m}^2 \text{s}^{-1}$)
D_l	diffusion coefficient in electrolyte ($\text{m}^2 \text{s}^{-1}$)
E_D	activation energy (J mol^{-1})
F	Faraday's constant (C mol^{-1})
G	The temperature gradient ($\times 10^3 \text{K m}^{-1}$)
h	heat convection coefficient ($\text{W m}^{-2} \text{K}^{-1}$)
j	current density ($\text{mol s}^{-1} \text{m}^{-2}$)
$\bar{l}_{dendrite}$	The normalized average dendrite length
M_η	electrochemical reaction-related constant (s^{-1})
M_σ	interfacial mobility ($\text{m}^3 \text{J}^{-1} \text{s}^{-1}$)
n_x, n_y	direction cosines of the outward normal vector at the boundaries
N	the number of dendrites
p^e	temperature-independent pre-exponent ($\text{m}^2 \text{s}^{-1}$)
\bar{q}_{de}	the normalized quantity of the electrodeposition
R	molar gas constant ($\text{J mol}^{-1} \text{K}^{-1}$)

R_d	the growth rate of dendrites
R_e	thermal conductivity in the electrode ($\text{W m}^{-1} \text{K}^{-1}$)
R_s	thermal conductivity in the electrolyte ($\text{W m}^{-1} \text{K}^{-1}$)
T	temperature (K)
T_0	ambient temperature (K)
U_j	open-circuit potential (V)
V	arbitrary volume
W_ξ	barrier height (J m^{-3})

Greek symbols

β	asymmetry factor
γ_N	interfacial energy (J m^{-2})
ϵ_R	emissivity constant
η	the overpotential (V)
κ_0	gradient energy coefficient (J m^{-1})
λ_e	conductivity of the electrode (S m^{-1})
λ_s	conductivity of the electrolyte solution (S m^{-1})
ξ	order parameter
ρ	mass density (kg m^{-3})
ρ_e	charge density (C m^{-1})
σ_R	Stefan-Boltzmann constant ($\text{W m}^{-2} \text{K}^{-4}$)
ϕ	electrostatic potential (V)

Massive experimental efforts [30–34] have also been implemented and most of them focused on the study of the effect of ambient temperatures on the dendritic growth process. The morphology evolution of the Li dendrite and the concurrent deterioration of the electrode cyclic ability were observed by their works. For instance, an inhomogeneous surface film was formed on the nickel substrate at a temperature of 40 °C, and the solid electrolyte interphase (SEI) layer suppressed the growth of the Li dendrite by changing into a uniform compact layer under high temperatures (60–80 °C) [35]. At a low temperature (−10 °C), Li was deposited on the surface of the negative electrode with applied charging currents and cut-off voltages, which presented a needle-like shape [36]. Recently, an experiment was performed by Yonemoto et al. [37] to study the temperature effects on the Li plating/stripping and showed that the cycling stability of the Li-metal anode can be enhanced by high temperatures. However, these experimental efforts are still at the stage where the thermal role is only characterized by the Li dendrite morphologies versus the imposed ambient temperature. In reality, however, the temperature is essentially contributed by the internal heat generation and the ambient temperature, and thus it is featured with a spatiotemporal evolution within the cells during operations.

In this article, we integrate our recently developed nonlinear phase-field Li-dendrite model [26] and a heat transfer model to computationally explore the thermal effect on the shape and size of Li dendrites during the growth process. The two models are linked by means of a temperature-dependent diffusion coefficient. The distributions of 1-D fields are investigated to validate the phase-field model. Then three levels of cases are applied in the 2-D system to progressively investigate the thermal effect on Li dendrites: (1) uniform ambient temperature, (2) temperature gradient along the charging direction, and (3) internal heat-induced spatially distributed temperature. A qualitative comparison between the numerical and the experimental results is implemented to validate the model in properly predicting the effect of the ambient temperature. The temperature gradient is applied to further explore the variations of the dendrite morphology and size. The internal heat is implemented to deeply investigate the thermal effect on the dendrite growth process. The computational work potentially offers valuable bases for further comprehensive studies of the temperature-dependent Li-dendrite growth process.

2. Theoretical framework**2.1. Phase-field model**

The current model is an extension of the nonlinear phase-field Li-dendrite model proposed by Chen [26]. And a brief outline of the model proposed by Chen is presented below to provide a self-contained analysis, and the complete description of the model can be found in Ref. [26]. Herein, consider the Li dendrite growth process, Li^+ cations in a liquid electrolyte (LiPF_6) transport through the SEI layer, and react with electrons e^- reduced to Li-atoms at the surface of the electrode. This process can be illustrated by $\text{Li}^+ + e^- \rightarrow \text{Li}$. And the schematic diagram of the Li dendrite growth process is shown in Fig. 1. To simplify the model, we make the following assumptions:

- (1) Reaction occurs in a binary dilute electrolyte.
- (2) Electrons are always provided at the surface of the electrode.

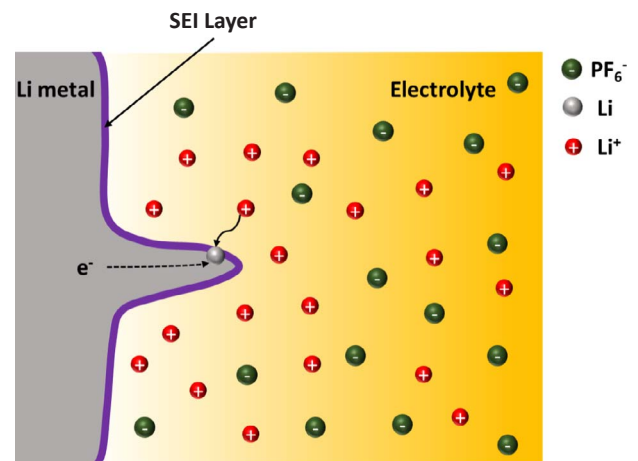


Fig. 1. Schematic diagram of a representative Li dendrite growth system. Red spheres: Li^+ ions; green spheres: PF_6^- ions; grey spheres: Li atoms. And the phase-field model which describes this process can be found in our published works [26]. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

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