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Analytical modeling of dislocation effect on diffusion induced stress in a cylindrical lithium ion battery electrode

Jia Li [a, b], Qihong Fang [a, b, *], Feng Liu [c], Youwen Liu [a, b]

[a] State Key Laboratory of Advanced Design and Manufacturing for Vehicle Body, Hunan University, Changsha, Hunan Province 410082, PR China
[b] College of Mechanical and Vehicle Engineering, Hunan University, Changsha, Hunan Province 410082, PR China
[c] State Key Laboratory for Powder Metallurgy, Central South University, Changsha, Hunan Province 410083, PR China

HIGHLIGHTS

- A coupled dislocation mechanical model for diffusion induced stress is established.
- A dislocation induced stress lowers tensile stress for galvanostatic & potentiostatic condition.
- The crack nucleation and propagation reduces at nanoscale cylindrical radius.
- Dislocation induced stress suppresses the crack nucleation.
- A new way reduces internal damage and improves battery life.

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ABSTRACT

This paper is theoretically suggested to describe the combined effects of diffusion induced stress and dislocation induced stress in a cylinder lithium ion battery electrode on the nucleation and propagation of cracks under galvanostatic or potentiostatic solute insertion and extraction. By the conventional assumption, we develop this model accounting for dislocation mechanics in a cylindrical electrode under axisymmetric diffusion induced stress, focusing on the dislocation and size effects on the magnitude and distribution of the combined DIS during galvanostatic or potentiostatic condition. The results show that dislocation induced stress can decrease tensile stress, and converts the state of stress from tensile to compressive. The trend of the crack nucleation and propagation can be prevented as the cylindrical particle radius drops down to nanoscale range. Dislocation induced stress suppressing the crack nucleation, however, provides a novel way of mitigating internal damage in a cylindrical lithium ion battery during cycling. It may be used in conjunction with the methods of nano-engineering to create microstructures tailored to maximize suppressing the crack nucleation, yielding new strategy to improve battery life and avoid failure.

1. Introduction

Lithium ion (Li-ion) batteries represent the subject of rapidly growing research efforts due to their outstanding physical properties, such as high energy density, superior rate capability and excellent cycling performance [1–3]. Li-ion batteries are now on the verge of wide-scale usage in automotive and mobile electronic devices, for instance electric vehicles (EV/HEV/PHEVs), notebooks and smart phones [4,5]. According to the materials perspective, silicon is one of the most promising candidates as electrodes for these Li-ion batteries, because it can provide a high energy and power density in nature [6–8]. Nevertheless, recent experiments show Li-ion insertion/extraction induced stresses in the silicon electrodes cause fracture [9] or morphological change [10], resulting in the capacity of the battery fading. In order to suppress or avoid fracture, a number of investigations in the last several decades have been conducted on this topic [8–12].

Many factors such as the concentration gradient effect and the saturation effect have been studied in recent years [13–15] during the process of charging/discharging, which could affect the distribution of diffusion induced stress (DIS). For example, Zhang et al. [16] studied three dimensional (3D) simulations of ellipsoidal

* Corresponding author. College of Mechanical and Vehicle Engineering, Hunan University, Changsha, Hunan Province 410082, PR China. Tel.: +86 73189822841; fax: +86 73188822330.
E-mail address: fangqh1327@hnu.edu.cn (Q. Fang).

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particles under intercalation, and suggested smaller sizes or larger aspect ratios reduce DIS. Cheng and co-workers [17] indicated the surface stress relieves DIS in nanoparticles. Using the modeling and experiment, Ye et al. [18] observed that Li-ion concentration gradient is greatly affected by temperature and decreases with the increasing temperature. Deshpande et al. [19] found DIS can cause the nucleation and growth of cracks leading to mechanical degradation of the active electrode materials. Han et al. [20] suggested that grain boundary can change the concentration distribution and also affects DIS. Recently, He et al. [21] studied the corresponding DIS in a symmetric layered electrode, and derived the variations of concentration-dependent elastic modulus on the Li-ion diffusion at the active layer. Several recent papers have studied DIS causing fracture using fracture mechanics [13,22].

In the above mentioned works, the researchers have separately studied the effect of DIS by various factors based on experimental research, computer simulations and theoretical models of physical properties of Li-ion batteries. However, few works have specifically considered the dislocation effect by Li-ion diffusion. Recently, Wei et al. [23] took into account the dislocation mechanics on DIS in a spherical particle electrode, and found edge dislocations by solute diffusion could relieve DIS. Hence, there is great interest in understanding dislocation induced stress to affect the physical properties of cylindrical particle electrode. The main aim of this paper is to build a theoretical model to study the combined effects of DIS and dislocation induced stress in the cylindrical Si electrode. In addition, the dislocation effect on the magnitude and distribution of DIS and the distinguishing differences between galvanostatic and potentiostatic controls will be discussed and calculated in detail.

2. Analytical model

Considering a cylindrical Li-ion battery electrode with the diameter $2R$ by the electrochemical reaction is suffering a flux of Li-ion into the Si cylindrical particle, as shown in Fig. 1(a). During charging, Li-ion by intercalation reaction is extracted from the cathode, and diffuses through the electrolyte towards the anode. During discharging, however, the electrochemical process of Li-ion extraction/intercalation is reversed [6–8]. The cathode is commonly made of a Lithium compound such as $LiFePO_4$, $LiMnO_2$, or $LiCoO_2$. The anode, on the other hand, consists mostly of graphite, silicon, or tin. The electrodes are separated by either a solid or a liquid, non-aqueous electrolyte Li-ion, which are allowed to transport from the positive electrode to the negative electrode during discharging and backwards upon charging process, as shown in Fig. 1(b).

The cylindrical particle electrode is assumed to be an isotropic and linearly elastic solid. Using the analogy between thermal stress and DIS [24,25], the stress and strain relationships in the cylindrical coordinate system can be expressed

$$\varepsilon_r = \frac{1}{E}[\sigma_r - \nu(\sigma_\theta + \sigma_z)] + \frac{1}{3}\Omega C(r,t) \tag{1}$$

$$\varepsilon_\theta = \frac{1}{E}[\sigma_\theta - \nu(\sigma_r + \sigma_z)] + \frac{1}{3}\Omega C(r,t) \tag{2}$$

where ε_r and ε_θ are the radial and tangential strains. σ_r and σ_θ are the radial and tangential stresses, respectively. E is Young's modulus, ν Poisson's ratio, Ω the partial molar volume of solute, and $C(r,t)$ the molar concentration of Li-ion.

Considering the electrode being a long wire, the axial strain may be negligible for the plane strain condition [19]

$$\varepsilon_z = 0 \tag{3}$$

For infinitesimally small deformation, the strain-displacement relations in the cylindrical coordinate system can be expressed by [26]

$$\varepsilon_r = \frac{du}{dr}, \quad \varepsilon_\theta = \frac{u}{r} \tag{4}$$

where u is the displacement in the radial direction.

Due to elastic deformation is a much faster process than atomic diffusion, and mechanical equilibrium is established [15]. In despite of body force, the expression of static mechanical equilibrium and the boundary conditions for the cylinder model may be expressed

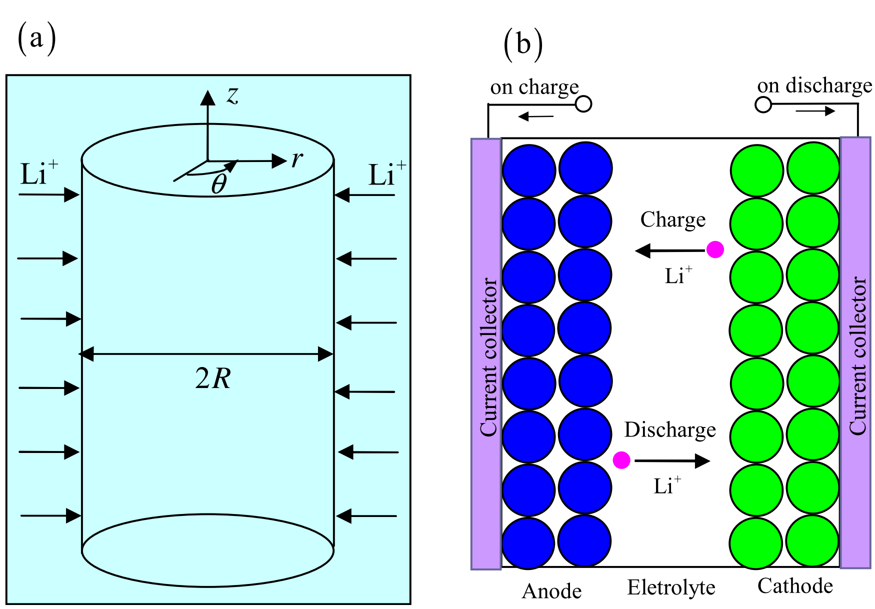

Fig. 1. Schematic illustration of Li-ion diffusion in a cylindrical particle electrode of diameter 2R modeled as diffusion uniformly at the surface of electrode during insertion/extraction (a). Schematic composition of a Li-ion battery (b).