Three-Dimensional Finite Element Study on Lithium Diffusion and Intercalation-Induced Stress in Polycrystalline LiCoO₂ using Anisotropic Material Properties

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Abstract

In current study, Lithium (Li) intercalation-induced stress of LiCoO₂ with anisotropic properties using three-dimensional microstructures has been studied systematically. Phase field method was employed to generate LiCoO₂ polycrystals with varying grain sizes. Li diffusion and stresses inside the polycrystalline microstructure with different grain size, grain orientation, and grain boundary diffusivity were investigated using finite element method. The results show the anisotropic mechanical properties and Li concentration dependent volume expansion coefficient have a very small influence on the Li chemical diffusion coefficients. The low partial molar volume of LiCoO₂ leads to this phenomenon. The anisotropic mechanical properties have a large influence on the magnitude of stress generation. Since the Young's modulus of LiCoO₂ along the diffusion pathway (a-b axis) is higher than that along c axis. The Li concentration gradient is larger along the diffusion pathway. Thus, for the same intercalation induced strain, the stress generation will be higher (~40%) than that with isotropic mechanical properties as discussed in our previous study

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(L. Wu, et al., J. Power Sources 299 (2015) 57). This work demonstrates the importance to include anisotropic property in the model.

Key words: LiCoO₂; modeling; grain boundary; stress generation; anisotropy.

1. Introduction

LiCoO_2 , as one of the cathode materials, has been widely used in lithium-ion batteries [1]. During the operation of lithium-ion batteries, lithium ions insert and extract from the host materials, causing the volume change of the host. The volume change will induce stresses and even lead to the mechanical failure. Therefore, one of the major tasks in lithium-ion batteries is to prevent mechanical degradation of electrodes during lithium insertion and extraction process. Previous studies shows LiCoO_2 [2], LiFePO_4 [3, 4] and LiMnO_2 [5] particles were fractured during cycling, leading to the capacity loss and power fade. Hence, it is necessary to understand the stress generation process during battery operations.

Many attentions have been attracted to explore the stress caused by lithium insertion in the battery material [6-11]. Christensen and Newman [12, 13] investigated the intercalation induced stress in lithium manganese oxide and carbon electrodes under galvanostatic conditions. Verbrugge and Cheng [14] simulated and analyzed the stress generation in a sphere electrode particle under galvanostatic conditions. Woodford et al. [15] derived the critical conditions of crack propagation in galvanostatic charging $\text{Li}_x\text{Mn}_2\text{O}_4$ particles based on fracture mechanics. However, most of the studies mentioned above used isotropic material properties and sphere-like shapes to simplify the problem. In their models, geometry effects and grain networks were not considered. The actual diffusion process in battery particles was very different than single spherical particle model. Experiment result [16, 17] has shown that secondary particles are a collection of single crystals separated by grain boundaries, indicating the majority of the primary particles inside the secondary particles are not in direct touch with the electrolyte. Therefore, it is important to study the intergranular diffusion in secondary particles.

Recently, several works have attempted to study the intergranular diffusion and stress generation in the cathode material. Han and Sastry [18] investigated the Li intercalation induced stress in elliptical particles by considering grain boundaries. In their study, they generated the polycrystal microstructure using Voronoi tessellation and didn't consider the grain orientation effects. Yamakawa et al. [9] simulated Li transport in polycrystalline LiCoO_2 with microstructures generated by phase field method. The model doesn't include the stress analysis caused by lithium intercalation. Our previous study [19] showed the effective Li diffusivity and stress generation are strongly affected by grain orientation, grain size and grain boundary diffusivity. In this study, the major contribution is to demonstrate the importance to include anisotropic property in the model. The anisotropic material properties including the diffusivity and Young's modulus will be used to study the grain orientation, grain size and grain boundary effects on effective Li diffusivity and its induced stress.

The paper will be organized as follows: (1) phase field method will be applied to generate polycrystal LiCoO_2 with different grain sizes. (2) The anisotropic effect of grain on Li chemical diffusion coefficient will be studied. (3) The stress generation in polycrystal with anisotropic mechanical properties will be investigated.

2. Calculation methods

2.1 Microstructures generation

In this study, four polycrystal microstructures were generated using phase field method. Each microstructure has different average grain size. The detailed description was in [19]. As shown in Fig. 1, different colors mean different grain orientations. The domain of the polycrystalline LiCoO_2 is $12.8 \times 12.8 \times 12.8 \mu\text{m}^3$. The average grain size of polycrystalline LiCoO_2 is 1.84 μm , 2.14 μm , 2.56 μm , and 2.7 μm , respectively. The simulated grain size of LiCoO_2

microstructure is consistent with the average grain size measured experimentally [20], which is about $1.5\ \mu\text{m}$ to $2.8\ \mu\text{m}$. The grain boundaries are assumed as thin layers, which is 10 nm in width. It is noted that in this study, the grain boundaries are treated as diffusion barriers with no actual geometric volumes. After the generation of polycrystalline LiCoO_2 , the chemical diffusion coefficient and stress generation were simulated by COMSOL Multiphysics.

(a)

(b)

(c)

(d)

Fig. 1 Generated polycrystalline LiCoO₂ microstructures. Different colors mean different grain orientations. Average grain size is (a) 1.84 μm ; (b) 2.14 μm ; (c) 2.56 μm ; and (d) 2.7 μm .

2.2 Li diffusion and stress generation

LiCoO₂ has a layered structure, in which all the lithium ions are located in a-b axis plane. It has been shown that LiCoO₂ has a two-dimensional diffusion pathway for lithium ions [21, 22]. Due to the higher energy barrier, it is very difficult for lithium ions to diffuse across the CoO₆ sheets. To consider the anisotropy of lithium diffusion in LiCoO₂ single crystals, an anisotropic diffusion tensor was used. The relationship between the local lithium diffusion and the global lithium transport was established based on the coordinates transformation (see Fig. 2).

The transport of lithium ions follows Fick's 2nd law with the influence of stress field, and is given by [23] :

$$\frac{\partial c}{\partial t} + \nabla \cdot \left(-D' \left(\nabla c - \frac{\Omega c}{RT} \nabla \sigma_h \right) \right) = 0 \quad (1)$$

where c is the lithium concentration inside the polycrystalline microstructure, D' is the anisotropic lithium diffusion tensor, Ω is the partial molar volume obtained from ref. [24], R is the gas constant, T is the absolute temperature and σ_h is the hydrostatic stress. The global anisotropic lithium diffusion tensor D' is related with the local diffusion tensor D ,

$$[D'] = [Q]^T [D] [Q] \quad (2)$$

where the transformation matrix Q relates the coordinate systems of local diffusion and global diffusion, as described in Fig. 2. α and γ shown in Fig. 2 are crystallographic orientation angles. Grain orientations are distributed randomly. In established coordinate systems, when α and γ are both 90°, the local 2D diffusion pathways are normal to the global Li influx direction, meaning the blockage of lithium ions. Due to the properties of the LiCoO₂, the local lithium diffusion tensor $[D]$ has the following form:

$$[D] = \begin{bmatrix} D_{self} & 0 & 0 \\ 0 & D_{self} & 0 \\ 0 & 0 & D_{self-caxis} \end{bmatrix} \quad (3)$$

where D_{self} is the self diffusion coefficient along lithium layers (which is a-b axis plane), and $D_{self-caxis}$ is the diffusion coefficient across the CoO_6 sheets (c axis).

In the model, the grain boundary is treated as a thin layer between two grains without geometric thickness. The mass transport of lithium ions across grain boundaries follows,

$$-\vec{n} \cdot D_{gb} \nabla c = \frac{D_{gb}}{d_{gb}} (c_u - c_d) \quad (4)$$

where D_{gb} is the lithium diffusivity in grain boundary; d_{gb} is the width which is assumed 10 nm. c_u and c_d are the lithium concentration across the grain boundary, respectively. We assume the diffusion coefficient of grain boundary has a relationship with lithium diffusion coefficient in single crystals,

$$D_{gb} = \beta D_{self} \quad (5)$$

where β is in the range of 0 and 1. $\beta=1$ indicates there is no grain boundary effect. In this study, β values were taken 0.01 and 1, which indicates small grain boundary diffusivity and large grain boundary diffusivity

Fig. 2 Schematics of local lithium diffusion coordinate system and the global lithium diffusion coordinate system. e_1 , e_2 and e_3 are local lithium diffusion coordinate system, while e_1' , e_2' , and e_3' are global lithium diffusion coordinate system. α and γ are crystallographic orientation angles. The global lithium influx is in $-e_1'$.

The chemical diffusivity of polycrystalline LiCoO_2 can be evaluated by [25],

$$D_{app} = -\frac{d(\ln(dc/dt))}{dt} \frac{4L^2}{\pi^2}, \quad \text{if} \quad t > L^2 / D_{app} \quad (6)$$

where L is the length of the domain in e_1' direction.

The boundary conditions used in simulating lithium diffusion in polycrystalline LiCoO_2 are listed in Table 1. It is noted that the surface in Table 1. is the polycrystal surface, not the LiCoO_2 crystallographic surface. For initial condition, the concentration of lithium ions in the microstructure is fixed at $x=0.6$ in Li_xCoO_2 . A constant lithium ion concentration is fixed at 0.61.

Intercalation induced stress in LiCoO₂ follows the modified Hooke's law with thermal analogy, and is given by,

$$\sigma_{ij} = C'_{ijkl} (\varepsilon_{kl} - \varepsilon_{kl}^L) \quad (7)$$

where ε_{kl} is strain, ε_{kl}^L is the strain induced by concentration change, σ_{ij} is stress, and C'_{ijkl} is the global stiffness matrix. The local stiffness matrix of the crystal was taken from [11]. The global stiffness matrix could be obtained by equation (2). ε_{kl}^L was derived from the concentration dependent lattice constants of Li_xCoO₂ in [24], as shown in Table 1 . Once the stress response is obtained, the hydrostatic stress can be calculated as $\sigma_h = (\sigma_x + \sigma_y + \sigma_z)/3$. To calculate the stress response, an incoming flux i_n/F was used, where i_n is the current density and F is the Faraday constant.

Table 2 Boundary conditions used in the model

	(100) surface	$\bar{(100)}$ surface	Other surfaces
Lithium diffusion	$c = \text{const. or } i_n/F$	$\vec{n} \cdot \nabla c = 0$	periodic
Intercalation stress	free	fixed	periodic

Table 3 Parameters used in the model

$D_{self} \text{ (cm}^2/\text{s)}$	1×10^{-9} [26]
$D_{self-caxis} \text{ (cm}^2/\text{s)}$	1×10^{-11} [27]
β	0.01 and 1

d_{gb} (nm)	10
c_{max} (mol/m ³)	51555 [28]
i_n (A/m ²)	2
T (K)	300
E_x, E_y (GPa)	321 [11]
E_z (GPa)	213 [11]
ϵ_x, ϵ_y	2.3×10^{-3} [24]
ϵ_z	-2.05×10^{-1} [24]

3. Results and discussion

3.1 Li Chemical diffusivity

The simulated Li chemical diffusivity D_{app} is shown in Fig.3. The Li chemical diffusivity in the microstructures is in the range of 9.4×10^{-10} cm²/s to 2.9×10^{-9} cm²/s for $\beta=0.01$ (small grain boundary diffusivity), and 1.80×10^{-9} cm²/s to 3.55×10^{-9} cm²/s for $\beta=1$ (large grain boundary diffusivity). Barker et al. measured the lithium diffusivity in Li_xCoO_2 0.1×10^{-9} cm²/s to 1.5×10^{-9} cm²/s when $0.3 < x < 0.85$ using electrochemical impedance spectroscopy [29]. In Jiang's work, the Li diffusivity of $LiCoO_2$ was reported 1×10^{-9} cm²/s using potentiostatic intermittent titration technique (PITT) [30]. The simulated chemical diffusion coefficient are consistent with experiments.

For both Fig. 3 (a) and (b), the chemical diffusion coefficient with anisotropic material properties is a little bit higher than that with isotropic properties. At higher grain crystallographic orientation angles, the chemical diffusion coefficient will be larger. This is because the local lithium diffusion pathway (a-b axis) is aligned with high orientation angles (α and γ are both 90°).

It can also be obtained that chemical diffusion coefficient is larger for large grains. At large grains, there are less grains in the domains, leading to less grain orientation mismatch. Compared with Fig. 3 (a) and (b), polycrystalline LiCoO_2 has smaller chemical diffusion coefficient with small grain boundary diffusivity, indicating grain boundary has block effect on lithium transport.

Compared with our previous work [19], the anisotropic mechanical properties and Li concentration dependent volume expansion coefficient have very small influence on the Li chemical diffusion coefficients. According to equation (1), the stress field influence on diffusion flux depends on the magnitude of partial molar volume. The low partial molar volume of LiCoO_2 leads to this phenomenon.

(a)

(b)

Fig. 3 Chemical diffusion coefficients with different orientation. (a) $\beta=0.01$. (b) $\beta=1$. Dashed lines are guide to the eyes for literature data. Solid lines are guide to the eyes for this work.

3.2 Stress generation

For both Fig. 4 (a) and (b), the hydrostatic stresses with anisotropic material properties are higher than that with isotropic properties. Hydrostatic stresses have greater values in larger grain systems. Large grain size indicates fewer grain boundaries and less orientation mismatch, leading to higher lithium concentration. Our simulated results are consistent with the mesoscale finite element analysis [31]. Additionally, energy release rate is higher in large grains, meaning fracture may happen at large grains first, which is in agreement with Zhao's result [32]. As shown in Fig. 4 (a), for small grain boundary diffusivity, stress levels are higher at high orientation angles. This

is because when local lithium transport is in alignment with global lithium influx, lithium ions are accumulated in grain boundary regions, causing stresses increase. While for large grain boundary diffusivity, as shown in Fig. 4 (b), stress levels decrease at large orientation angles because of less concentration gradient near grain boundary areas. As the crystallographic orientation angles reach 90°, lithium ions can migrate without the blockage of grain boundaries, leading to smaller stress. Compared Fig. 4 (a) and Fig. 4 (b), the diffusion coefficient of the grain boundary has opposite effect on stresses. Smaller grain boundary diffusivity causes higher stress. It can also be evidenced by Fig. 5. In Fig. 5 (a), small grain boundary diffusivity causes a slower lithium ion diffusion because of the blockage effect. For large grain boundary diffusivity ($\beta=1$), it has a smaller concentration gradient, resulting less stresses than that of small grain boundary diffusivity case ($\beta=0.01$), which is shown in Fig. 5 (b).

(a)

(b)

Fig. 4 The hydrostatic stresses on different grain sizes and orientation angles. (a) $\beta=0.01$ (b) $\beta=1$. Dashed lines are guide to the eyes for literature data. Solid lines are guide to the eyes for this work.

The hydrostatic stresses with different grain sizes, grain orientations and grain boundary diffusivities has the same trend as the previous work [19], as shown in Fig. 4. Although the anisotropic mechanical properties have very small influence on the Li chemical diffusion coefficients, it does have large influence on the stress generation. For LiCoO_2 , the Young's modulus along the diffusion pathway (a-b axis) is higher than that along c axis. The Li concentration gradient is larger along the diffusion pathway. Thus, for the same intercalation induced strain, the stress generation will be higher (~40%) than that with isotropic mechanical properties.

Fig. 5 (a) Lithium concentration profiles and (b) Hydrostatic stresses of polycrystalline LiCoO_2 with $1.84 \mu\text{m}$ grain size and different grain boundary diffusivities. The plane shown is a cut plane at $z=6.4 \mu\text{m}$, $t=50 \text{ s}$, and orientation angle 30° .

4. Conclusions

In this work, the three-dimensional Li diffusion and stress generation in polycrystalline LiCoO_2 with anisotropic material properties have been studied using finite element method. The influence of grain networks on lithium diffusion and its induced stress has been investigated. The conclusions are given as the following:

- (1) The anisotropic mechanical properties and Li concentration dependent volume expansion coefficient have very small influence on the Li chemical diffusion coefficients. The low partial molar volume of LiCoO_2 leads to this phenomenon.
- (2) The hydrostatic stress with various grain sizes, grain orientations and grain boundary diffusivities has the same trend as that with isotropic mechanical properties.
- (3) The anisotropic mechanical properties have large influence on the stress generation. For LiCoO_2 , the Young's modulus along the diffusion pathway (a-b axis) is higher than that along c axis. The Li concentration gradient is larger along the diffusion pathway. Thus, for the same intercalation induced strain, the stress generation will be higher ($\sim 40\%$) than that with isotropic mechanical properties.

5. Acknowledgement

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6. Data Availability

The raw/processed data required to reproduce these findings cannot be shared at this time as the data also forms part of an ongoing study.

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