



공학석사 학위논문

# A coupled electrochemical-mechanical analysis of unidirectional structural battery composites using multiscale modeling

멀티스케일 모델링을 이용한 단방향 구조 전지 복합재의 전기화학적-기계적 연계 해석

2022년 8월

서울대학교 대학원

재료공학부

장 동 원

# A coupled electrochemical-mechanical analysis of unidirectional structural battery composites using multiscale modeling

Advisor: Woong-Ryeol Yu

by

Dongwon Jang

# 2022

Department of Materials Science and Engineering Graduated School Seoul National University

# A coupled electrochemical-mechanical analysis of unidirectional structural battery composites using multiscale modeling

멀티스케일 모델링을 이용한 단방향 구조 전지 복합재의 전기화학적-기계적 연계 해석

지도 교수 유 웅 열

이 논문을 공학석사 학위논문으로 제출함 2022년 6월

> 서울대학교 대학원 재료공학부 장 동 원

장동원의 공학석사 학위논문을 인준함 2022년 6월

위 육	신 장	<u></u>	(인)
부위	원장	유웅열	(인)
위	원	이명규	(인)

# Abstract

Structural battery composites (SBCs) are multifunctional composites that can serve as both an energy storage and external load supporter. Carbon fiber and epoxy-based structural electrolyte with excellent mechanical properties used for SBCs serve as the electrode and transport Li-ion, respectively. Establishing a simplified model is essential to predict the effective electrochemical and mechanical behaviors of large-scale SBCs. Herein, we carried out a coupled electrochemical-mechanical analysis using multiscale modeling for optimum design of large-scale SBCs. A yarn scale model was built using electrochemical and mechanical homogenization methods. In a parallel effort, a filament scale model was visually modeled without any homogenization method. Then, the two models were analyzed and compared. A similarity between the yarn scale and the filament scale was verified by using 3D shape descriptors (compactness and cubeness) and volumeaveraged method. These results provide a theoretical understanding of electrochemical and mechanical behaviors of SBCs in multiscale.

**Keywords:** Structural battery composites, coupled electrochemicalmechanical analysis, multiscale modeling, homogenization Student Number: 2020-29422

# Contents

Abstract	i
Contents	iii
List of Tables	V
List of Figures	v

1. Introduction	1
1.1. Structural battery composites	1
1.2. Previous studies of electrochemical-mechanical simulation for SBCs	1
1.3. Research objectives	2

2. Multiscale modeling	4
2.1. Yarn scale	6
2.1.1. Electrochemical model	6
2.1.2. Mechanical model	10
2.2. Filament scale	11
2.2.1. Electrochemical model	11
2.2.2. Mechanical model	13
2.3. Geometrical and physical parameters	14

3. Results and Discussion	18
3.1. Electrochemical and mechanical analysis of yarn scale	18
3.2. Electrochemical and mechanical analysis of filament scale	21
3.3. Comparison between yarn scale and filament scale	24
3.3.1. Electrochemical property comparison	24

Iechanical property comparison   28
1echanical property comparison

4. Conclusion	
Appendix A	
Reference	
Korean abstract	

## **List of Tables**

Table 1 Parameters of geometry.

 Table 2 Parameters of electrochemical model.

Table 3 Parameters of mechanical model.

Table 4 Comparison of compactness between YS and FS over time.

Table 5 Comparison of cubeness between YS and FS over time.

# **List of Figures**

**Figure 1** Illustration of two different scale models for the unidirectional SBCs. (a) unidirectional large-scale SBCs in YS, (b) unidirectional large-scale SBCs in FS, (c) repeated unit of unidirectional large-scale SBCs in YS, (d) repeated unit of unidirectional large-scale SBCs in FS, (e) 2D simulation model of repeated unit in YS and (f) 2D simulation model of repeated unit in FS.

**Figure 2** Normalized Li concentration distribution over time in YS. (Left color bar : yarn electrode, right color bar : PE)

**Figure 3** Mechanical analysis of YS model at t = 1800 s. (a) Von mises stress, (b)  $\sigma_{xx}$ , (c)  $\sigma_{yy}$ , (d)  $\sigma_{zz}$  and (e) volumetric strain.

**Figure 4** Normalized Li concentration distribution over time in FS. (Left color bar : carbon fiber, right color bar : PE)

**Figure 5** Mechanical analysis of FS model at t = 1800 s. (a) Von mises stress, (b)  $\sigma_{xx}$ , (c)  $\sigma_{yy}$ , (d)  $\sigma_{zz}$  and (e) volumetric strain.

Figure 6 Comparison of voltage profile between YS and FS.

Figure 7 Comparison of volumetric strain between YS and FS over time via surface average function.

## **Chapter 1. Introduction**

#### 1.1. Structural battery composites

Currently, interest in Li-ion batteries (LIBs) is growing due to the growth of the electric vehicle market and environmental problems [1-3]. LIBs used in electric transportation have difficulties in fire hazards due to the use of liquid electrolyte and increased weight of the entire system due to LIBs' own weight [4-7]. As an alternative to solving the above problems, SBCs have been introduced that can serve as the same energy storage as LIBs and can be used as the outer frame of transportation with external load support [8-10]. The important materials used in SBCs are carbon fiber which acts as the electrode and has excellent mechanical properties, and non-flammable epoxy-based structural electrolyte (SE) that can transport Li-ion while having good mechanical properties [11, 12]. The fabrication of the SBCs using the above materials lags far behind their conceptual theory due to experimental limitations, but Asp et al. recently built a developed model of SBCs [13].

# 1.2. Previous studies of electrochemical-mechanical simulation for SBCs

Following the above interest, the development of electrochemical-mechanical simulation for SBCs is in progress based on previous studies on simulation of LIBs. Li et al. investigated the stress in positive particles of LIBs according to charging rates and structural parameters [14]. Based on a multiscale approach, Lee et al.

developed an electrochemical-mechanical modeling framework to study stress generation in LIBs [15]. The similarity of the two different scale models in LIBs was verified by Wu et al. through electrochemical and mechanical analysis [16]. Furthermore, Xu et al. conducted a multiphysics modeling to analyze for electrochemical and mechanical behaviors in a single carbon fiber micro-battery [17]. Carlstedt et al. investigated the effects of state of charge on elastic properties of 3D SBCs and proposed modeling framework of laminated SBCs to account for electrochemical-mechanical coupling effects [18, 19]. Yin et al. and Hong et al. proposed a modeling framework for modified carbon fiber anode to improve the electrochemical properties and analyzed structural parameters for modified carbon fiber electrodes [20, 21]. Previous studies showed that the frameworks applied to SBCs were visually modeled with individual carbon fiber filaments.

#### **1.3. Research objectives**

When manufacturing large-scale SBCs to be used for the outer frame of transportation with carbon fiber yarn, the numerous carbon fiber filaments inevitably have the form of yarn. Also, establishing a simplified model is essential to predict the effective electrochemical and mechanical behaviors of large-scale SBCs. A yarn scale (YS) modeling framework, which can be linked with a filament scale (FS) to simulate large-scale SBCs, has not been conducted.

Herein, we carried out a coupled electrochemical-mechanical analysis using multiscale modeling for optimum design of large-scale SBCs. First, the YS model was built using homogenization methods based on the porous electrode theory and the Mori-Tanaka model [22, 23]. In a parallel effort, the FS model was visually modeled without any homogenization method. Then, electrochemical and mechanical analyses were performed at each scale. Finally, the similarity of these two scales in the electrochemical aspect was analyzed using the 3D shape descriptors. The similarity of these two scales in the mechanical aspect was analyzed using the volume-averaged method.

## **Chapter 2. Multiscale modeling**

Unidirectional SBCs are laminated structures, in which positive electrode (PE), separator, and carbon fiber are stacked in order, and the remaining space is filled with SE. LiFePO<sub>4</sub> (LFP) was used as an active material of PE. The PE was modeled as the porous electrode in which active material, binder, carbon black, and SE are mixed in a certain ratio [22]. On the other hand, carbon fiber was used as an active material of negative electrode without the above mixing process. Based on the experimental design of SBCs [13], large-scale SBCs in YS and FS were illustrated by using these materials in **Figure 1**(a) and (b). Since computational time and cost are limited in simulating the whole large-scale SBC, we extracted repeated unit of large-scale SBCs as shown in **Figure 1**(c) and (d). In the repeated unit, geometric parameters of each component were summarized in **Table 1**. Next, we designed 2D simulation models of repeated unit for convenience as shown in **Figure 1**(e) and (f). In both models, one specific carbon fiber of each yarn was modeled as a current collector that plays a role in exchanging electrons between an external circuit and active material due to high electrical conductivity [24].



**Figure 1** Illustration of two different scale models for the unidirectional SBCs. (a) unidirectional large-scale SBCs in YS, (b) unidirectional large-scale SBCs in FS, (c) repeated unit of unidirectional large-scale SBCs in YS, (d) repeated unit of unidirectional large-scale SBCs in FS, (e) 2D simulation model of repeated unit in YS and (f) 2D simulation model of repeated unit in FS.

#### 2.1. Yarn scale

#### 2.1.1. Electrochemical model

In the YS, a carbon fiber yarn consisted of numerous carbon fiber filaments and SE. It was regarded as the porous electrode in which two continuous phases coexist.

#### (a) Electrolyte domain

In the electrolyte domain of porous electrode, the conservation of mass is described by the Nernst-Plank equation as below:

$$f_l \frac{\partial c_l}{\partial t} + \nabla \cdot \mathbf{N}_l^Y = R_l \tag{1}$$

where  $f_i$  is the volume fraction of electrolyte,  $c_i$  is the Li-ion concentration in the electrolyte, t is the time,  $N_i^{\gamma}$  is the Li-ion flux of electrolyte in YS, and  $R_i$  is the mass source of Li-ion in the electrolyte. In conventional battery conditions, convection, one of the three main mass transport mechanisms in the electrolyte, is not considered. So Li-ion flux is given by diffusion and electromigration:

$$\mathbf{N}_{l}^{Y} = -D_{l}^{eff} \nabla c_{l} + \frac{\mathbf{i}_{l}^{Y} t_{+}}{F}$$
<sup>(2)</sup>

where  $D_l^{eff}$  is the effective electrolyte diffusivity,  $\mathbf{i}_l^{\gamma}$  is the current density of electrolyte in YS,  $t_+$  is the Li-ion transference number, and F is the Faraday constant.  $\mathbf{i}_l^{\gamma}$  is described with Ohm's law and Li-ion concentration gradient:

$$\mathbf{i}_{l}^{Y} = -\sigma_{l}^{eff} \nabla \phi_{l} + \left(\frac{2\sigma_{l}^{eff} RT}{F}\right) \left(1 + \frac{\partial \ln f}{\partial \ln c_{l}}\right) (1 - t_{+}) \nabla \ln c_{l}$$
(3)

where  $\sigma_l^{eff}$  is the effective electrolyte conductivity,  $\phi_l$  is the electrolyte potential,

R is the gas constant, and f is the electrolyte activity coefficient.

In porous electrode like YS, transport properties should be calibrated because of the effects of porosity. So effective transport properties are given by:

$$\sigma_l^{eff} = f_l^{\gamma} \sigma_l, \quad \sigma_s^{eff} = f_s^{\gamma} \sigma_s, \quad D_l^{eff} = f_l^{\gamma} D_l \tag{4}$$

where  $\sigma_i$  is the electrolyte conductivity,  $\sigma_s^{eff}$  is the effective electrical conductivity,  $f_s$  is the volume fraction of active material,  $\sigma_s$  is the electrical conductivity,  $D_i$  is the electrolyte diffusivity, and  $\gamma$  is the Bruggeman constant, which has a value of 1.5 for spherical particles such as LFP [25]. On the other side, carbon fiber as active material has cylindrical geometry. For non-spherical particles like carbon fiber, different appropriate  $\gamma$  should be applied [26].

The conservation of charge in the electrolyte is related with Li intercalation induced current density i:

$$\nabla \cdot \mathbf{i}_{l}^{Y} = a_{s} i \tag{5}$$

where  $a_s$  is the surface of active material per unit volume. For spherical particles  $a_s = \frac{3f_s}{r_p}$ , where  $r_p$  is the radius of active material. On the other hand, for cylindrical particles  $a_s = \frac{2f_s}{r_f}$ , where  $r_f$  is the radius of carbon fiber.

#### (b) Electrode domain

In the electrode domain of porous electrode, the conservation of mass is described by Fick's law for diffusion:

$$\frac{\partial c_s}{\partial t} + \nabla \cdot \mathbf{N}_s^{\mathrm{Y}} = 0 \tag{6}$$

$$\mathbf{N}_{s}^{Y} = -D_{s} \nabla c_{s} \tag{7}$$

where  $c_s$  is the Li concentration of active material,  $N_s^{\gamma}$  is the Li flux of active material in YS, and  $D_s$  is the diffusion coefficient of active material. The current density in the electrode domain is described by Ohm's law:

$$\mathbf{i}_{s}^{Y} = -\sigma_{s}^{eff} \nabla \phi_{s} \tag{8}$$

where  $\mathbf{i}_{s}^{\gamma}$  is the current density of active material in YS and  $\phi_{s}$  is the potential of active material. The conservation of charge in active material is related to Li intercalation induced current density:

$$\nabla \cdot \mathbf{i}_s^Y = -a_s i \tag{9}$$

#### (c) Charge transfer kinetics

The electrochemical reaction occurs at the interface between active material and electrolyte, which is governed by the Butler-Volmer equation:

$$i = i_0 \left[ \exp\left(\frac{\alpha_a F \eta}{RT}\right) - \exp\left(\frac{-\alpha_c F \eta}{RT}\right) \right]$$
(10)

where  $i_0$  is the exchange current density,  $\alpha_a$  and  $\alpha_c$  are the anodic and cathodic charge transfer coefficients,  $\eta$  is the overpotential, and T is the temperature.  $i_0$ and  $\eta$  are calculated as below:

$$i_{0} = F(k_{c})^{\alpha_{a}}(k_{a})^{\alpha_{c}}(c_{s,\max} - c_{s,surf})^{\alpha_{a}}(c_{s,surf})^{\alpha_{c}}\left(\frac{c_{l}}{c_{l,0}}\right)^{\alpha_{a}}$$
(11)

$$\eta = \phi_s - \phi_l - E_{eq} \tag{12}$$

where  $k_a$  and  $k_c$  are the anodic and cathodic rate constant,  $c_{s,max}$  is the maximum Li concentration in the active material,  $c_{s,surf}$  is the Li concentration on the active material surface,  $c_l$  and  $c_{l,0}$  are the Li-ion concentration in the electrolyte and the initial Li-ion concentration in the electrolyte, and  $E_{eq}$  is the open circuit potential of active material. The governing equations of reaction kinetics are the same for both YS and FS. The boundary conditions for the electrochemical model in YS are given by:

$$\frac{\partial c_s}{\partial r} = 0$$
 at  $r = 0$  (13a)

$$-D_s \frac{\partial c_s}{\partial r} = \frac{i}{F}$$
 at  $r = r_p$  and  $r = r_f$  (13b)

$$c_s = c_{s,0}$$
 and  $c_l = c_{l,0}$  at  $t = 0$  (13c)

$$n \cdot N_l^{\gamma} = 0$$
 at  $x = 0$ ,  $x = W$ ,  $y = 0$  and  $y = L_c + L_s + L_a$  (13d)

$$n \cdot \mathbf{i}_s^{Y} = 0$$
 and  $n \cdot \mathbf{i}_l^{Y} = 0$  at  $x = 0$ ,  $x = W$  and  $y = L_c + L_s + L_a$  (13e)

$$-n \cdot \mathbf{i}_{s}^{Y} = I_{app} \quad \text{at} \quad y = 0 \tag{13f}$$

$$\phi_s = 0$$
 at the current collector surface (13g)

where  $I_{app}$  is the applied current density based on C-rate of 1C when SBCs are charged.

#### 2.1.2. Mechanical model

Like a porous electrode in the electrochemical model, a carbon fiber yarn was considered as a composite electrode. Methods based on volume average for predicting homogenized mechanical properties of composite include Voigt model, Reuss model, and Mori-Tanaka model [27]. Among them, the Mori-Tanaka model, which is the most common and highly accurate model, was applied to the yarn.

Assuming battery components are linear-elastic materials, the macroscopic stress is governed by stress equilibrium:

$$\nabla \cdot \sigma^{Y} = 0 \tag{14}$$

where  $\sigma^{\gamma}$  is the stress in YS and body force is neglected. The macroscopic stress tensor is given by:

$$\sigma_{ij}^{Y} = C_{ijkl}^{Y}(\varepsilon_{kl} - \varepsilon^{Y}\delta_{kl})$$
(15)

where  $C_{ijkl}^{\gamma}$  is the effective stiffness tensor of yarn,  $\varepsilon_{kl}$  is the strain tensor,  $\varepsilon^{\gamma}$  is the Eigen strain tensor of yarn resulting from Li intercalation/deintercalation of carbon fiber, and  $\delta_{kl}$  is the Kronecker delta. Based on volume average,  $\varepsilon^{\gamma}$  is given by:

$$\varepsilon^{\gamma} = f_{s}\beta_{ij}M(c_{avg} - c_{ref})$$
(16)

where  $\beta_{ij}$  is the swelling tensor of carbon fiber, M is the molar mass of Li,  $c_{avg}$  is the average Li concentration in the active material, and  $c_{ref}$  is the strain-free reference concentration. The calculation process of  $C_{ijkl}^{Y}$  using MATLAB was found

in **Appendix A**. The boundary conditions for the mechanical model in YS are given by:

$$u=0$$
 at  $y=0$  and  $y=L_c+L_s+L_a$  (17a)

$$u \cdot n = 0$$
 at  $x = 0$  and  $x = W$  (17b)

where u is the displacement and n is the unit normal vector.

#### 2.2. Filament scale

The FS model was visually modeled as carbon fiber filaments were gathered in the form of closed packing. Furthermore, SE and carbon fiber filaments were depicted separately.

#### 2.2.1. Electrochemical model

(a) Electrolyte domain

In the electrolyte domain, the conservation of mass is described by the Nernst-Plank equation as below:

$$\frac{\partial c_l}{\partial t} + \nabla \cdot \mathbf{N}_l^F = 0 \tag{18}$$

where  $\mathbf{N}_{l}^{F}$  is the Li-ion flux of electrolyte in FS. The Li-ion flux in the electrolyte domain is given by:

$$\mathbf{N}_{l}^{F} = -D_{l}\nabla c_{l} + \frac{\mathbf{i}_{l}^{F}t_{+}}{F}$$
(19)

where  $\mathbf{i}_{l}^{F}$  is the current density of electrolyte in FS.  $\mathbf{i}_{l}^{F}$  is described with Ohm's

law and Li-ion concentration gradient:

$$\mathbf{i}_{l}^{F} = -\sigma_{l}\nabla\phi_{l} + \left(\frac{2\sigma_{l}RT}{F}\right)\left(1 + \frac{\partial\ln f_{\pm}}{\partial\ln c_{l}}\right)\left(1 - t_{\pm}\right)\nabla\ln c_{l}$$
(20)

The conservation of charge in the electrolyte is given by:

$$\nabla \cdot \mathbf{i}_l^F = 0 \tag{21}$$

#### (b) Electrode domain

In the electrode domain of FS, the conservation of mass is described by Fick's law for diffusion:

$$\frac{\partial c_s}{\partial t} + \nabla \cdot \mathbf{N}_s^F = 0 \tag{22}$$

$$\mathbf{N}_{s}^{F} = -D_{s}\nabla c_{s} \tag{23}$$

where  $\mathbf{N}_{s}^{F}$  is the Li flux of active material in FS. The current density in the electrode domain is described by Ohm's law:

$$\mathbf{i}_{s}^{F} = -\sigma_{s} \nabla \phi_{s} \tag{24}$$

where  $\mathbf{i}_{s}^{F}$  is the current density of active material in FS. The conservation of charge in active material is given by:

$$\nabla \cdot \mathbf{i}_s^F = 0 \tag{25}$$

The boundary conditions for the electrochemical model in FS are given by:

$$n \cdot \mathbf{N}_s^F = 0$$
 at current collector surface (26a)

$$n \cdot \mathbf{N}_s^F = \frac{i}{F}$$
 at electrolyte-carbon fiber interface (26b)

$$n \cdot \mathbf{N}_l^F = 0$$
 at  $x = 0$ ,  $x = W$ ,  $y = 0$  and  $y = L_c + L_s + L_a$  (26c)

$$n \cdot \mathbf{N}_{l}^{F} = \frac{i}{F}$$
 at electrolyte-carbon fiber interface (26d)

$$n \cdot \mathbf{i}_s^F = 0$$
 and  $n \cdot \mathbf{i}_l^F = 0$  at  $x = 0$ ,  $x = W$  and  $y = L_c + L_s + L_a$  (26e)

$$n \cdot \mathbf{i}_s^F = -i$$
 and  $n \cdot \mathbf{i}_l^F = i$  at electrolyte-carbon fiber interface (26f)

$$-n \cdot \mathbf{i}_s^F = I_{app} \quad \text{at} \quad y = 0 \tag{26g}$$

$$\phi_s = 0$$
 at current collector surface (26h)

#### 2.2.2. Mechanical model

Carbon fiber and SE have mechanical properties of transverse isotropic and isotropic respectively. Stress equilibrium in FS is given by:

$$\nabla \cdot \sigma^F = 0 \tag{27}$$

where  $\sigma^{F}$  is the stress in FS and body force is neglected. The stress tensor of carbon fiber and SE is given by:

$$\sigma_{ii}^{F} = C_{iikl}^{F} (\varepsilon_{kl} - \varepsilon^{F} \delta_{kl})$$
(28)

where  $C_{ijkl}^{F}$  is the stiffness tensor of each component calculated by Hooke's law and  $\varepsilon^{F}$  is the Eigen strain tensor of carbon fiber resulting from Li intercalation/deintercalation.

$$\varepsilon^{F} = \beta_{ij} M(c_{s} - c_{ref})$$
<sup>(29)</sup>

The calculation process of  $C_{ijkl}^{F}$  was implemented by MATLAB using the mechanical properties of each component. The boundary conditions for the mechanical model in FS are given by:

$$u = 0$$
 at  $y = 0$  and  $y = L_c + L_s + L_a$  (30a)

$$u \cdot n = 0$$
 at  $x = 0$  and  $x = W$  (30b)

#### 2.3. Geometrical and physical parameters

The parameters required for the electrochemical model and mechanical model were summarized in **Table 1**, **Table 2**, and **Table 3** respectively. We used the built-in properties of LFP and brought the properties of IMS65 carbon fiber. Also, the open circuit potential data of carbon fiber was replaced by experimental data at slow cycling (0.3C) in a carbon fiber-Li metal coin cell [24]. The diffusivity of cation and anion in SE was assumed to be equal. Both simulation models were solved using finite element method (FEM) software COMSOL Multiphysics 5.6 under plane strain condition.

 Table 1 Parameters of geometry.

ParametersValueLength of positive electrode/ $L_c$ (µm)50Length of separator/ $L_s$ (µm)6.28Length of negative electrode/ $L_a$ (µm)150Width of repeated unit/ $W$ (µm)50	
Length of positive electrode/ $L_c$ (µm)50Length of separator/ $L_s$ (µm)6.28Length of negative electrode/ $L_a$ (µm)150Width of repeated unit/ $W$ (µm)50	Reference
Length of separator/ $L_s$ (µm)6.28Length of negative electrode/ $L_a$ (µm)150Width of repeated unit/ $W$ (µm)50	
Length of negative electrode/ $L_a$ (µm)150Width of repeated unit/ $W$ (µm)50	
Width of repeated unit/ $W$ (µm) 50	
Radius of LFP particle/ $r_p$ (µm) 0.1	
Radius of carbon fiber/ $r_f$ (µm) 2.5	[24]

Parameters	Domain/ material	Value	Reference
Volume fraction of active material $f$	PE	0.4	
volume indefion of derive indefinity $f_s$	Yarn	0.755	
	PE	0.5	
Volume fraction of electrolyte/ $f_l$	Separator	0.5	
	Yarn	0.245	
Maximum Li concentration in active	2LFP	21190	
material/ $C_{s,max}$ (mol/m <sup>2</sup> )	Carbon fiber	16800	[19]
Initial Li concentration in active material	/LFP	21190	
$c_{s,0}$ (mol/m <sup>3</sup> )	Carbon fiber	168	
Initial Li-ion concentration in electrolyte $c_{l,0}$ (mol/m <sup>3</sup> )	SE	1000	
Diffusion coefficient of active material/ $D_s$	LFP	3.2×10 <sup>-13</sup>	
$(m^{2}/s)$	Carbon fiber	1×10 <sup>-13</sup>	[24]
Diffusion coefficient of electrolyte/ $D_{l}$ (m <sup>2</sup> /s)	SE	2.66×10 <sup>-12</sup>	[12, 28, 29]
Electrical conductivity/ $\sigma$ (S/m)	LFP	91	
	Carbon fiber	69000	[24]
Electrolyte conductivity/ $\sigma_i$ (S/m)	SE	2×10 <sup>-2</sup>	[12]
Transport number/ $t_+$	SE	0.363	
Reaction rate constant $k$ k	PE	4.5×10 <sup>-12</sup>	[30]
Reaction rate constants $\kappa_c, \kappa_a$	Yarn	4.2×10 <sup>-12</sup>	[30]
Bruggeman constant/ v	PE	1.5	[25]
Bruggeman constant, y	Yarn	1.7	[26]
Applied current density/ $I_{app}$ (A/m <sup>2</sup> )		10.11	[31, 32]
Temperature/ $T$ (K)	All domain	298	
Faraday constant/ F (C/mol)	All domain	96500	
Gas constant/ $R$ (J/mol · K)	All domain	8.314	

 Table 2 Parameters of electrochemical model.

Parameters	Material	Value	Reference
Longitudinal modulus/ $E_{zz}$ (GPa)	Carbon fiber	290	[11]
Transverse modulus/ $E_{xx}$ , $E_{yy}$ (GPa)	Carbon fiber	21.8	[11]
Poisson's ratio/ $v_s$	Carbon fiber	0.2	
Longitudinal shear modulus/ $G_{yz}$ , $G_{zx}$ (GPa)	Carbon fiber	12.5	[11]
Transverse shear modulus/ $G_{xy}$ (GPa)	Carbon fiber	9.08	
Elastic modulus/ $E_l$ (GPa)	SE	0.53	[12]
Poisson's ratio/ $v_l$	SE	0.33	
Longitudinal swelling coefficient/ $\beta_{zz}$ (m <sup>3</sup> /kg)	Carbon fiber	1.718×10 <sup>-4</sup>	[19, 20, 33]
Transverse swelling coefficient/ $\beta_{xx}$ , $\beta_{yy}$ (m <sup>3</sup> /kg)	Carbon fiber	8.589×10 <sup>-4</sup>	[19, 20, 33]
The molar mass of Li (g/mol)		7	
Strain-free reference concentration/ $c_{ref}$ (mol/m <sup>3</sup> )	Carbon fiber	168	

 Table 3 Parameters of mechanical model.

### **Chapter 3. Results and Discussion**

#### 3.1. Electrochemical and mechanical analysis of yarn scale

Figure 2(a)-(d) shows the average Li concentration distribution in YS with time. The Li concentration decreased in PE and increased in varn electrode during charge. In yarn electrode, since the Li intercalation started from the carbon fiber filaments close to the PE, the Li concentration of Yarn 1 was higher than that of Yarn 3. The difference in the Li concentration between Yarn 1 and Yarn 3 became larger with time. Figure 3(a) shows the Von mises stress due to the Li intercalation in YS. By comparing Figure 2(b) and Figure 3(a), it could be seen that the Von mises stress distribution showed the same tendency as the Li concentration distribution. When the stress components were examined separately,  $\sigma_{xx}$ ,  $\sigma_{yy}$ , and  $\sigma_{zz}$  were all negative values, indicating compressive stress (Figure 3(b)-(d)).  $\sigma_{xx}$  and  $\sigma_{yy}$  with relatively small absolute values contributed little to the Von mises stress, whereas  $\sigma_{\rm\scriptscriptstyle zz}\,$  with relatively large absolute values was a major factor of the Von mises stress due to the large longitudinal modulus of yarn. Figure 3(e) shows the volumetric strain, which means that volume expansion due to Li intercalation occurred because the value of volumetric strain was positive. It could be seen that the volumetric strain also showed the same tendency as the Li concentration distribution in **Figure 2**(b).



**Figure 2** Normalized Li concentration distribution over time in YS. (Left color bar : yarn electrode, right color bar : PE)



**Figure 3** Mechanical analysis of YS model at t = 1800 s. (a) Von mises stress, (b)  $\sigma_{xx}$ , (c)  $\sigma_{yy}$ , (d)  $\sigma_{zz}$  and (e) volumetric strain.

#### 3.2. Electrochemical and mechanical analysis of filament scale

**Figure 4**(a)-(d) shows the Li concentration distribution in FS with time. The Li concentration in the carbon fiber filaments increased with time overall. The Li intercalation started from the carbon fiber filaments close to the PE, so the Li concentration of Yarn 1 was higher than that of Yarn 3. As time went on, the difference in the Li concentration between Yarn 1 and Yarn 3 became larger. After the electrochemical reaction occurred at the interface between carbon fiber filament and electrolyte, Li entered the center of each carbon fiber filament by diffusion, so it should have had a circular Li concentration gradient in carbon fiber filaments. However, since the carbon fiber filaments were arranged in closed packing with a limited SE, the mass transfer did not occur effectively in the yarn electrode, and thus a circular Li concentration fiber filaments did not appear.

The Von mises stress distribution, which appeared due to volume expansion by Li intercalation, was governed by Li concentration in the carbon fiber filaments as shown in **Figure 4**(b) and **Figure 5**(a). Furthermore, when numerous carbon fiber filaments were gathered to have the shape of yarn, contact with each carbon fiber filament was inevitable. The stress concentration occurred at these contact parts and had the same stress as in **Figure 5**(b) and (c). The main factor having the Von mises stress distribution as shown in **Figure 5**(a) was the  $\sigma_{zz}$  in **Figure 5**(d) because of extremely high longitudinal modulus of carbon fiber. In **Figure 5**(e), it could be seen that the carbon fiber filaments expanded during Li intercalation because the value of volumetric strain was positive. The volumetric strain by stress concentration at the contact parts and the volumetric strain by Li intercalation appeared together.



**Figure 4** Normalized Li concentration distribution over time in FS. (Left color bar : carbon fiber, right color bar : PE)



**Figure 5** Mechanical analysis of FS model at t = 1800 s. (a) Von mises stress, (b)  $\sigma_{xx}$ , (c)  $\sigma_{yy}$ , (d)  $\sigma_{zz}$  and (e) volumetric strain.

#### 3.3. Comparison between yarn scale and filament scale

#### 3.3.1. Electrochemical comparison

To confirm the electrochemical similarity of two different scale models, we compared voltage-time graphs between YS and FS. The voltage-time graphs showed no significant difference as shown in **Figure 6**. However, comparing the voltage-time graphs was difficult to validate the similarity between YS and FS because the Li concentration distributions of two different scale models were slightly different.



Figure 6 Comparison of voltage profile between YS and FS.

Therefore, we used a geometric analysis that can quantify 3D shape called compactness [34, 35]. This analysis could indicate that how much a given 3D shape differs from the most compact shape, a sphere, as a numeric value between 0 and 1. Compactness ( $C^{z}$ ) based on the geometric moment is obtained as follows:

$$C^{z} = \frac{3^{5/3}}{5(4\pi)} \times \frac{(\mu_{0,0,0})^{5/3}}{\mu_{2,0,0} + \mu_{0,2,0} + \mu_{0,0,2}}$$
(31)

where

Central moment, 
$$\mu_{p,q,r} = \iiint_{S} (x - x_c)^p (y - y_c)^q (z - z_c)^r dxdydz$$
 (32)

The central moment consists of centroid and moment as follow:

Centroid, 
$$(x_c, y_c, z_c) = \left(\frac{m_{1,0,0}}{m_{0,0,0}}, \frac{m_{0,1,0}}{m_{0,0,0}}, \frac{m_{0,0,1}}{m_{0,0,0}}\right)$$
 (33)

Moment, 
$$m_{p,q,r} = \iiint_{S} x^{p} y^{q} z^{r} dx dy dz$$
 (34)

Another 3D shape descriptor called cubeness based on the geometric moment was also used. This analysis could indicate that how much a given 3D shape differs from the most compact shape, a cube, as a numeric value between 0 and 1 [35, 36]. Cubeness ( $C^{M}$ ) is calculated as follows:

$$C^{M} = \frac{3}{8} \times \frac{Volume^{4/3}}{\min_{\alpha,\beta \in [0,2\pi]} \iiint_{S(\alpha,\beta)} \max\left\{|x|, |y|, |z|\right\} dx dy dz}$$
(35)

where  $S(\alpha,\beta)$  indicates that the shape S is rotated along the x-axis by  $\alpha$  angle and along the y-axis by  $\beta$  angle. To calculate compactness and cubeness using Equations (31)-(35) in MATLAB, x component, y component, and z component were set as x-coordinate, y-coordinate, and value of Li concentration respectively. In YS, since the yarn was treated as porous electrode, the Li concentration was observed in all yarn domain. However, since the Li concentration should only appear in the carbon fiber domain, we selectively extracted the value of Li concentration from YS.

Table 4 shows the comparison of compactness between YS and FS over time. At 0 s, all yarn had same the compactness in both scales due to the initial Li concentration condition. Overall, the compactness of both scales in all yarn decreased with time. This was because  $\mu_{2,0,0}$  and  $\mu_{0,2,0}$  were not changed with time but  $\mu_{0,0,2}$ , which was the second central moment of Li concentration, increased with time. The compactness values for all yarn were similar until 1800 s, but showed a difference after 1800 s. And when considering the total amount of Li concentration in each yarn domain, the similarity in the compactness of Yarn 1 was greater than the similarity in the compactness of Yarn 3. Table 5 shows the comparison of cubeness between YS and FS over time. At 0 s, all yarn also had the same cubeness in both scales due to the initial Li concentration condition. The cubeness values for Yarn 1 were similar until the end of charge, while the cubeness values for Yarn 2 and Yarn 3 were similar until 1800 s, and showed a difference after 1800 s. Therefore, the similarity of cubeness for Yarn 1 was greater than the similarity of cubeness for Yarn 2 and Yarn 3. A reasonable reason for these results was that the difference in the transport properties of two different scales increased with time and distance away from PE.

Scale		YS			FS	
Domain	Yarn 1	Yarn 2	Yarn 3	Yarn 1	Yarn 2	Yarn 3
Time			C	Z		
0 s	0.1549	0.1549	0.1549	0.1549	0.1549	0.1549
900 s	0.1533	0.1547	0.1548	0.1526	0.1543	0.1545
1800 s	0.1534	0.1531	0.1538	0.1525	0.1534	0.1541
2700 s	0.1432	0.1503	0.1518	0.1443	0.1527	0.1544
3600 s	0.1349	0.1406	0.1495	0.1435	0.1484	0.1543

Table 4 Comparison of compactness between YS and FS over time.

Table 5 Comparison of cubeness between YS and FS over time.

Scale		YS			FS	
Domain	Yarn 1	Yarn 2	Yarn 3	Yarn 1	Yarn 2	Yarn 3
Time			С	М		
0 s	0.1241	0.1241	0.1241	0.1241	0.1241	0.1241
900 s	0.1562	0.1447	0.1427	0.1573	0.1458	0.1436
1800 s	0.2188	0.1746	0.1637	0.2182	0.1787	0.1680
2700 s	0.2619	0.2132	0.1771	0.2636	0.2231	0.1868
3600 s	0.1587	0.2430	0.1849	0.1606	0.2737	0.2005

#### 3.3.2. Mechanical comparison

To compare the mechanical similarity between YS and FS, we used the volumeaveraged method. This method is given by:

$$\langle \varepsilon \rangle_i = \frac{1}{V_i} \int_{V_i} \varepsilon_i dV_i$$
(36)

where  $\langle \varepsilon \rangle_i$  is the volume-averaged strain of a specific phase,  $V_i$  is the total volume of a specific phase, and  $\varepsilon_i$  is the strain of a specific phase. The volume-averaged strain of two-phase composites about yarn is related by:

$$\langle \varepsilon \rangle = f_s \langle \varepsilon \rangle_s + f_l \langle \varepsilon \rangle_l \tag{37}$$

where  $\langle \varepsilon \rangle$  is the volume-averaged strain of yarn,  $\langle \varepsilon \rangle_s$  is the volume-averaged strain of carbon fiber filaments, and  $\langle \varepsilon \rangle_l$  is the volume-averaged strain of SE. The result of the above method can be computed using the "volume average" function built in COMSOL Multiphysics 5.6 [37]. However, the "volume average" function was not available because the simulation models were 2D. To solve this, since the 2D models were infinitely long in the z-direction, it could be substituted by the "surface average" function.

**Figure 7** shows the comparison of volume-averaged volumetric strain via the "surface average" function. The similarity of volumetric strains in YS and FS was good until 1800 s and decreased over time. Since the volumetric strain was governed by the Li concentration, the similarity of volumetric strain had a similar tendency to the results of comparing the Li concentration shape through compactness and cubeness. Furthermore, the difference in volumetric strain was larger than the difference in compactness and cubeness because the strain field inside the carbon

fiber, which was affected by stress concentration by the adjacent carbon fiber filaments other than the Li concentration, was not considered in YS.



Figure 7 Comparison of volumetric strain between YS and FS over time via surface average function.

## **Chapter 4. Conclusion**

In this study, a coupled electrochemical-mechanical analysis of unidirectional SBCs using multiscale modeling to simulate large-scale SBCs was carried out. The multiscale of SBCs was developed into the YS model using porous electrode theory and Mori-Tanaka theory, and the FS model using visual modeling, respectively. The observations and findings through simulation results of two different scale models were summarized below:

- 1. The electrochemical and mechanical behaviors of yarn electrode in YS could be adequately expressed with a relatively short computational time.
- 2. The FS model showed detailed electrochemical and mechanical behaviors considering the contact effect of carbon fiber filaments.
- In terms of electrochemical and mechanical aspects, the similarity between the YS model and the FS model showed good agreement in limited time and distance.
- 4. The mechanical similarity between the YS model and the FS model showed a similar tendency to the electrochemical similarity, but the mechanical similarity was lower than the electrochemical similarity because the strain field influenced by adjacent carbon fiber filaments was not considered in YS.

#### Appendix A. Stiffness matrix of yarn using Mori-Tanaka model

Each yarn was regarded as a unidirectional composite consisting of isotropic SE (matrix) and aligned infinitely long carbon fiber filaments (inclusions) with transversely isotropic properties. To calculate the homogenized stiffness tensor of yarn, the Mori-Tanaka model was applied [38]. For the single-inclusion case, the volume-averaged strain of carbon fiber is linked with the volume-averaged strain of SE as follows:

$$\langle \varepsilon \rangle_s = T_{ii} \langle \varepsilon \rangle_l \tag{A1}$$

where  $T_{ij}$  is the strain concentration tensor.  $T_{ij}$  is expressed by:

$$T_{ij} = [I + S : (C_l^{-1} : C_s - I)]^{-1}$$
(A2)

where I is the identity tensor, S is the Eshelby's tensor that depends on the geometry of inclusion and the Poisson's ration of matrix,  $C_I$  is the stiffness tensor of SE,  $C_s$  is the stiffness tensor of carbon fiber. In Voigt notation, S for the infinite long fiber in z-direction is given by: [39]

$$S = \begin{bmatrix} S_{1111} & S_{1122} & S_{1133} & 0 & 0 & 0 \\ S_{2211} & S_{2222} & S_{2233} & 0 & 0 & 0 \\ S_{3311} & S_{3322} & S_{3333} & 0 & 0 & 0 \\ 0 & 0 & 0 & 2S_{2323} & 0 & 0 \\ 0 & 0 & 0 & 0 & 2S_{1313} & 0 \\ 0 & 0 & 0 & 0 & 0 & 2S_{1212} \end{bmatrix}$$
(A3)

where

$$S_{1111} = S_{2222} = \frac{1}{2(1-v_l)} \left[ \frac{3}{4} + \frac{(1-2v_l)}{2} \right]$$
(A4)

$$S_{1122} = S_{2211} = \frac{1}{2(1-v_l)} \left[ \frac{1}{4} - \frac{(1-2v_l)}{2} \right]$$
(A5)

$$S_{1133} = S_{2233} = \frac{v_l}{2(1 - v_l)}$$
(A6)

$$S_{3311} = S_{3322} = S_{3333} = 0 \tag{A7}$$

$$S_{2323} = S_{1313} = \frac{1}{4} \tag{A8}$$

$$S_{1212} = \frac{1}{2(1-v_l)} \left[ \frac{1}{4} + \frac{(1-2v_l)}{2} \right]$$
(A9)

With using S, the effective stiffness tensor of yarn is obtained by:

$$C_{ijkl}^{Y} = [f_s C_s : T_{ij} + (1 - f_s)C_l] : [f_s T_{ij} + (1 - f_s)I]^{-1}$$
(A10)

#### Reference

- Meng, J., et al., An overview and comparison of online implementable SOC estimation methods for lithium-ion battery. IEEE Transactions on Industry Applications, 2017. 54(2): p. 1583-1591.
- Zubi, G., et al., *The lithium-ion battery: State of the art and future perspectives.* Renewable and Sustainable Energy Reviews, 2018. 89: p. 292-308.
- Bai, Y., et al., *Energy and environmental aspects in recycling lithium-ion batteries: Concept of Battery Identity Global Passport.* Materials Today, 2020. 41: p. 304-315.
- 4. Zeng, Z., et al., *Non-flammable electrolytes with high salt-to-solvent ratios for Li-ion and Li-metal batteries.* Nature Energy, 2018. **3**(8): p. 674-681.
- 5. Balakrishnan, P., R. Ramesh, and T.P. Kumar, *Safety mechanisms in lithiumion batteries.* Journal of power sources, 2006. **155**(2): p. 401-414.
- Pham, H.Q., et al., Non-flammable organic liquid electrolyte for highsafety and high-energy density Li-ion batteries. Journal of Power Sources, 2018. 404: p. 13-19.
- Zackrisson, M., L. Avellán, and J. Orlenius, *Life cycle assessment of lithiumion batteries for plug-in hybrid electric vehicles–Critical issues.* Journal of Cleaner Production, 2010. 18(15): p. 1519-1529.
- Asp, L.E., et al., *Structural battery composites: a review.* Functional Composites and Structures, 2019. 1(4): p. 042001.
- Johannisson, W., D. Zenkert, and G. Lindbergh, *Model of a structural battery and its potential for system level mass savings.* Multifunctional Materials, 2019. 2(3): p. 035002.
- Carlstedt, D. and L.E. Asp, *Performance analysis framework for structural battery composites in electric vehicles.* Composites Part B: Engineering, 2020. 186: p. 107822.
- 11. Duan, S., et al., *Determination of transverse and shear moduli of single carbon fibres.* Carbon, 2020. **158**: p. 772-782.
- Schneider, L.M., et al., *Bicontinuous electrolytes via thermally initiated polymerization for structural lithium ion batteries.* ACS Applied Energy Materials, 2019. 2(6): p. 4362-4369.
- Asp, L.E., et al., *A structural battery and its multifunctional performance.* Advanced Energy and Sustainability Research, 2021. 2(3): p. 2000093.

- Li, Q., et al., Stress and its influencing factors in positive particles of lithium-ion battery during charging. International Journal of Energy Research, 2021. 45(3): p. 3913-3928.
- Lee, Y.K., J. Song, and J. Park, *Multi-scale coupled mechanical*electrochemical modeling for study on stress generation and its impact on multi-layered electrodes in lithium-ion batteries. Electrochimica Acta, 2021. 389: p. 138682.
- Wu, B. and W. Lu, A consistently coupled multiscale mechanical– electrochemical battery model with particle interaction and its validation. Journal of the Mechanics and Physics of Solids, 2019. 125: p. 89-111.
- Xu, J., G. Lindbergh, and J. Varna, *Multiphysics modeling of mechanical* and electrochemical phenomena in structural composites for energy storage: Single carbon fiber micro-battery. Journal of Reinforced Plastics and Composites, 2018. **37**(10): p. 701-715.
- Carlstedt, D., E. Marklund, and L.E. Asp, *Effects of state of charge on elastic properties of 3D structural battery composites.* Composites Science and Technology, 2019. 169: p. 26-33.
- Carlstedt, D., et al., *Electro-chemo-mechanically coupled computational modelling of structural batteries.* Multifunctional Materials, 2020. 3(4): p. 045002.
- Yin, S., et al., Fabrication and multiphysics modeling of modified carbon fiber as structural anodes for lithium-ion batteries. Journal of Power Sources, 2020. 476: p. 228532.
- Hong, Z., et al., *Multiphysics modeling framework for composite structural batteries with modified carbon fibers as electrodes.* Composites Communications, 2021. 27: p. 100853.
- Fuller, T.F., M. Doyle, and J. Newman, *Simulation and optimization of the dual lithium ion insertion cell.* Journal of the Electrochemical Society, 1994.
  141(1): p. 1.
- Mori, T. and K. Tanaka, Average stress in matrix and average elastic energy of materials with misfitting inclusions. Acta metallurgica, 1973. 21(5): p. 571-574.
- Kjell, M.H., et al., *Electrochemical characterization of lithium intercalation* processes of PAN-based carbon fibers in a microelectrode system. Journal of The Electrochemical Society, 2013. **160**(9): p. A1473.

- Landesfeind, J., et al., *Tortuosity determination of battery electrodes and separators by impedance spectroscopy.* Journal of The Electrochemical Society, 2016. **163**(7): p. A1373.
- Vadakkepatt, A., et al., Bruggeman's exponents for effective thermal conductivity of lithium-ion battery electrodes. Journal of the Electrochemical Society, 2015. 163(2): p. A119.
- Tian, W., et al., Numerical evaluation on mechanical properties of shortfiber-reinforced metal matrix composites: Two-step mean-field homogenization procedure. Composite Structures, 2016. 139: p. 96-103.
- Chintapalli, M., et al., *Relationship between conductivity, ion diffusion, and transference number in perfluoropolyether electrolytes.* Macromolecules, 2016. 49(9): p. 3508-3515.
- Zadin, V. and D. Brandell, *Modelling polymer electrolytes for 3D-microbatteries using finite element analysis.* Electrochimica acta, 2011. 57: p. 237-243.
- Taslimi Taleghani, S., B. Marcos, and G. Lantagne, *Modeling and simulation* of a commercial graphite–LiFePO4 cell in a full range of C-rates. Journal of Applied Electrochemistry, 2018. 48(12): p. 1389-1400.
- Liu, P., et al., Computational modeling of heterogeneity of stress, charge, and cyclic damage in composite electrodes of Li-Ion batteries. Journal of The Electrochemical Society, 2020. 167(4): p. 040527.
- 32. Dasari, H. and E. Eisenbraun, *Predicting capacity fade in silicon anodebased Li-ion batteries.* Energies, 2021. **14**(5): p. 1448.
- Jacques, E., et al., *Expansion of carbon fibres induced by lithium intercalation for structural electrode applications.* Carbon, 2013. 59: p. 246-254.
- 34. Žunić, J., K. Hirota, and C. Martinez-Ortiz. *Compactness measure for 3d shapes*. in *2012 International Conference on Informatics, Electronics & Vision (ICIEV)*. 2012. IEEE.
- An, Y., et al., *Quantitative evaluation of the three-dimensional deployment behavior of a shape memory polymer antenna.* Smart Materials and Structures, 2018. 27(10): p. 105007.
- 36. Martinez-Ortiz, C. and J. Žunić. *Measuring cubeness of 3d shapes*. in *Iberoamerican Congress on Pattern Recognition*. 2009. Springer.
- 37. Schutzeichel, M.O.H., T. Kletschkowski, and H.P. Monner, Microscale

*Thermal Modelling of Multifunctional Composite Materials Made from Polymer Electrolyte Coated Carbon Fibres Including Homogenization and Model Reduction Strategies.* Applied Mechanics, 2021. **2**(4): p. 739-765.

- 38. Liu, L. and Z. Huang, *A note on Mori-Tanaka's method.* Acta Mechanica Solida Sinica, 2014. **27**(3): p. 234-244.
- 39. Mura, T., *Micromechanics of defects in solids*. 2013: Springer Science & Business Media.

## Korean abstract

구조 배터리 복합재는 에너지 저장 및 외부 하중 지지체 역할을 할 수 있는 다기능 복합재이다. 구조 배터리 복합재에 사용되는 기계적 물성이 우수한 탄소 섬유 및 에폭시 기반 구조 전해질은 각각 전극 역할과 리튬 이온을 수송한다. 대규모 구조 배터리 복합재의 효과적인 전기화학적 및 기계적 거동을 예측하기 위해 단순화된 모델을 설정하는 것이 중요하다. 여기에서, 우리는 대규모 구조 배터리 복합재의 최적 설계를 위해 다중 규모 모델링을 이용한 전기화학적-기계적 연계 해석을 수행하였다. 전기 화학적 및 기계적 균질화 방법을 이용하여 원사 규모 모델을 구축하였다. 동시에, 필라멘트 규모 모델은 균질화 방법 없이 시각적으로 모델링 되었다. 그 후, 각 규모 모델본 전기화학적 및 기계적 분석을 진행하였고, 두 다른 규모 모델의 유사도를 비교하였다. 3차원 형상 기술자(조밀 함과 입방체)와 부피 평균 방법을 이용하여 원사 규모와 필라멘트 규모 의 유사성을 검증하였다. 이러한 결과는 다중 규모에서 구조 배터리 복 합재의 전기화학적 및 기계적 거동에 대한 이론적인 이해를 제공한다.

핵심어: 구조 배터리 복합재, 전기화학적-기계적 연계 해석, 다중 규모 모델링, 균질화

학번:2020-29422