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An electro-chemo-thermo-mechanical coupled three-dimensional computational framework for lithium-ion batteries

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Abstract

Thermal and mechanical effects play a vital role in determining the electrochemical behavior of lithium-ion batteries (LIBs). Non-uniform temperature distribution and mechanical deformation can result in uneven electrochemical states, leading to spatially varying aging rates that significantly shorten cell lifetime. In order to improve simulation accuracy and thus the quality of computational battery design optimization, it is therefore essential to capture these coupled phenomena in a simulation model of a full battery cell. In this work, an electro-chemo-thermo-mechanical coupled framework is proposed to simulate LIBs in the three-dimensional space. In this new framework, a recently proposed one-dimensional electrochemical model, which includes the impact of mechanical deformation and local lithiation state on the effective transport properties of the charged species, is coupled with a three-dimensional thermomechanical model. A unique coupling scheme is proposed to handle information exchange between these two models. This framework allows us to accurately and efficiently study the behavior of three-dimensional cells with realistic geometry and resolve the spatial variation of interested fields. Two commercial cells are studied to show the performance of the newly proposed battery simulation framework.

Keywords mechanical deformation · electro-chemo-thermo-mechanical model · porosity change · DualFoil model · lithium-ion battery · full-cell simulation

1 Introduction

The development of elaborated numerical models is essential for understanding the complex multi-domain phenomena involved in a battery cell. For applications such as electric vehicles or stationary energy storage systems, which use hundreds to tens of thousands of lithium-ion cells, sophisticated numerical algorithms are required to simulate battery performance and aging in a computationally efficient manner. The findings obtained from such models can be used to improve battery design, e.g., to optimize energy density, power output, or lifespan, and to build advanced battery-management systems (BMS) that predict battery behavior, precisely control individual cells, and balance electrical loadings to minimize aging and ensure reliable and safe operation.

The so-called DualFoil model developed by Newman and his co-workers provides a rigorous description of the physical processes of battery systems based on the concentrated solution theory and porous electrode theory [2–5]. The DualFoil model is capable of capturing diffusion in lithium-insertion materials, ionic transport in the electrolyte, and interfacial reactions. It outputs various battery state variables, including voltage, potential, and concentration profiles. This model has been modified to account for thermal effects [6,7] and other phenomena, such as side-reactions, film formation, and dendrite growth [8–11]. Recently, the DualFoil model was extended to account for mechanical effects by allowing porosity and species transport distance to change depending on the mechanical load and local swelling of the electrode material [12].

The DualFoil model and its modified versions are one-dimensional (1D) models oriented along an axis perpendicular to the different layers in a battery cell, i.e., cathode, separator, and anode. We will refer to this axis as the sandwich-layer through-direction (SLTD). Such treatment is sufficient for studying electrochemistry and thermal effects occurring
Figure 1: Illustration of two solution domains for the new 3D ECTM model, adapted from ref. [14]. (a) A fine finite element mesh of the jellyroll of an 18650 cell with \( n_{\text{TM}} \) elements, on which the thermomechanical model is solved for the spatially varying temperature and stress fields. (b) A coarse mesh with each element spatially covering multiple thermomechanical elements. Each coarse element is associated with a 1D electrochemical sub-cell. The electrochemical behavior of the whole jellyroll is described by connecting all sub-cells, with a total number of \( n_{\text{EC}} \), in parallel with identical voltage. The sum of the current output from sub-cells is enforced to match the applied total current \( I \) with \( I = \sum_{i=1}^{n_{\text{EC}}} I_i \). Volume-averaged quantities are used to exchange information between the thermomechanical model and the electrochemical model.

In lithium-ion batteries (LIBs), mechanical deformation can arise both from a volume change within the cell components, such as intercalation induced swelling of the active material, thermal expansion, film growth due to side reactions, and externally applied mechanical loadings [19–22]. Particularly, in battery cells that contain high energy density electrode materials, such as Silicon or Germanium, the large volume change of the active material during lithium (Li) intercalation can cause fracture or pulverization of the electrodes [23–26]. For these material systems, mechanical effects predominantly define the electrochemical performance and lifetime of the battery cells. For battery cells made with conventional electrode materials, such as graphite and LiCoO₂, the volume change of the active material during Li intercalation is comparatively small [27–29]. However, it may still impact the electrochemical performance of a battery cell due to a change of the local porosity and because of an increase (decrease) of the distance that the charged species need to traverse as the electrodes expand (contract) [12, 20, 30]. These effects are typically cyclic and mostly reversible. However, irreversible processes, e.g., due to side-reactions such as Li-plating, may also occur and need to be considered in the definition of the optimal mechanical pressure applied to a battery cell [31].

In this work, we focus on cells made with conventional electrode materials. Compared to the number of 3D battery models that include thermal effects [14–17, 32–36], battery models that consider the mechanical impact on the electrochemical performance of LIBs in the 3D dimensional setting are scarce. In [37], a one-way coupled electro-chemo-thermo-mechanical (ECTM) model is proposed to study the stress level due to Li intercalation and thermal expansion for one sandwich layer, but the authors did not investigate how mechanical deformation affects the electrochemical behavior of LIBs. A 3D implementation of an extended DualFoil model including mechanical deformation, porosity change, and thermal expansion is presented in [38] and used to study coupling effects in a sandwich layer geometry. In a different work [39], the same authors investigate these effects by explicitly resolving the geometry of the pores and particles inside of the electrodes and separator. However, both models are computationally expensive and make it challenging to study the electrochemical behavior on the full-cell level.

To overcome these limitations, in this work, an efficient 3D ECTM coupled framework is proposed that allows studying the interplay of different physical processes occurring at multiple scales up to the cell level. For this purpose, we adapt the mesh mapping technique described in [14]. As illustrated in Fig. 1, a fine mesh is used to compute the homogenized thermomechanical behavior of the cell. This allows us to obtain a high spatial resolution for the temperature and displacement fields. To simulate the cell’s electrochemical response, we generate a coarse mesh with each element representing a 1D electrochemical sub-cell. The sub-cell is discretized in the SLTD, which distinguishes the two
electrodes and the separator. In our simulation, we do not explicitly create the coarse 3D mesh as shown in Fig. 1(b). Instead, a lookup table is generated to group multiple thermomechanical elements to represent the coarse mesh. The overall electrochemical behavior of the jellyroll is obtained by connecting all the sub-cells in parallel, as shown in Fig. 1. In this framework, the sub-cells' parameters and states can be specified independently and updated in parallel on a high-performance computer. It allows us to assign different parameters (e.g., porosity and thickness) to each sub-cell to account for a non-uniform material distribution in the jellyroll. A two-way coupling scheme is used to exchange information between the thermomechanical and the electrochemical part of the simulation through volume-averaged quantities and projected stress.

2 Model Description

In this section, we describe the proposed coupled framework in detail. First, a 3D thermomechanical model formulated in the large deformation setting is presented. Next, a recently proposed mechanically coupled 1D DualFoil model [12] is summarized, which accounts for the change of the local porosity and the distance that charged species cross from one electrode to the other. We then describe the two-way information exchange scheme between the electrochemical model and the thermomechanical model.

2.1 Thermomechanical model

The finite strain theory in continuum mechanics is used to characterize the homogenized mechanical response of a battery. Interested readers are directed to [40] for details. Using the finite strain theory allows us to accurately describe the elastic deformation, intercalation-induced volume change, and thermal expansion, respectively. The deformation of a battery is denoted by \( \varphi \) with \( \varphi = X + u \), where \( X \) is the position vector of a point inside the battery in the reference configuration and \( u \) is the displacement vector of that point. The deformation gradient \( F = \partial X / \partial u = I + \omega u \) is a quantity to characterize the shape change of a solid body with \( I \) as a second order identity tensor. We consider a multiplicative decomposition of \( F \) with

\[
F = F_{\text{elastic}} F_{\text{swelling}} F_\theta \quad \text{with} \quad F_{\text{swelling}} = I + \omega n \otimes N
\]  

(1)

where \( F_{\text{elastic}}, F_{\text{swelling}}, \) and \( F_\theta \) describe the elastic deformation, intercalation-induced volume change, and thermal expansion, respectively. The term \( \omega \) in (1) is a volume change ratio due to Li-intercalation. \( F_{\text{swelling}} \) describes the anisotropic volume change occurring in the SLTD, as the strain is found to be negligible in the two in-plane directions compared to the SLTD with three-dimensional digital image correlation technique in [41]. The thermal expansion coefficients for the electrodes and the separator are on the order of \( 10^{-5} \text{ K}^{-1} \) [42]. Considering that the operation temperature range of a battery is typically less than 60 K, thermal-induced volume change is smaller than 0.06%. This value is much smaller compared to the reversible intercalation-induced volume change of around 2.0% [27]. Based on the above comparison, we neglect thermal-induced expansion by setting \( F_\theta = I \). This assumption is supported by [37]. The deformation and the temperature fields \( \varphi \) and \( \theta \) are obtained by solving the balance of linear momentum and the heat equation

\[
\text{Div} [P] = 0 \quad \text{and} \quad \rho C_p \frac{\partial \theta}{\partial t} + \nabla \cdot (-\kappa \nabla \theta) = \dot{q}
\]  

(2)

together with the properly imposed Dirichlet and Neumann boundary conditions. In Eq. (2), \( P \) is the first Piola-Kirchhoff stress with \( P = \partial F W \). For the strain energy density \( W \), we assume a Neo-Hookean relation

\[
W(F) = \frac{\mu}{2} \left( \text{tr}(C_{\text{elastic}}) - 3 - 2 \ln \mathcal{J}_{\text{elastic}} \right) + \frac{\lambda}{2} \left( \mathcal{J}_{\text{elastic}} - 1 \right)^2,
\]  

(4)

where \( \mu \) and \( \lambda \) are elastic material parameters, \( C_{\text{elastic}} \) is the right elastic Cauchy-Green tensor with \( C_{\text{elastic}} = F_{\text{elastic}}^T F_{\text{elastic}} \), and \( \mathcal{J}_{\text{elastic}} \) is the determinant of \( F_{\text{elastic}} \), respectively. With (4), the Cauchy stress \( \sigma \) is computed as

\[
\sigma = \frac{PF^T}{\mathcal{J}} = \frac{1}{1 + \omega} \left( \lambda \left( \mathcal{J}_{\text{elastic}} - 1 \right) I + \frac{\mu}{\mathcal{J}_{\text{elastic}}} \left( F_{\text{elastic}} F_{\text{elastic}}^T - I \right) \right).
\]  

(5)

\(^1\)The lookup table can be created either based on the spatial coordinates, where thermomechanical elements in close proximity are grouped together, or based on the state variables, where thermomechanical elements with similar temperature and projected stress are grouped together. The latter case allows us to dynamically increase or decrease the total number of electrochemical sub-cells based on the evolution of state variables during charge/discharge to improve the efficiency of the electrochemical simulation.
In Eq. (5), $\dot{q}$ is calculated based on Eq. (19) from the electrochemical model. The Eqs. (2) and (3) are solved with an in-house finite element code based on the deal.II library \cite{43}. Interested readers are directed to Ref. \cite{43} for details of the finite element method.

2.2 Mechanically coupled 1D DualFoil model

The DualFoil model and its modified versions describe the charge-transfer kinetics at the electrode-electrolyte interfaces, mass transfer and potential variation in both the active solid electrode materials and the liquid electrolyte based on the porous electrode and concentrated solution theory. The governing equations of this model are well described in the literature \cite{2, 4}. In order to capture thermal effects, carefully determined temperature dependent material parameters and a model for the various sources of heat generation are required. A comprehensive description of the individual heat generation rates in an electrochemical cell is given in \cite{7}. This work employs a mechanically coupled DualFoil model \cite{12}, which accounts for the change of porosity and distance of charged species transport due to Li intercalation and externally applied mechanical loading. In the following, we give a short outline on how these effects are modelled. A summary of the resulting equations is given in Table I.

Mechanical coupling. The effective electrochemical properties in Table I such as diffusivity and conductivity, depend on the porosity of the electrodes. For this, we assume the common Bruggeman’s relationship \cite{3}

$$D_{e, \text{eff}} = D_{e} \epsilon_{\text{eff}}^\alpha, \quad \kappa_{e, \text{eff}} = \kappa_{e} \epsilon_{\text{eff}}^\alpha, \quad \kappa_{s, \text{eff}} = \kappa_{s} \epsilon_{\text{eff}}^\alpha, \quad \sigma_{\text{eff}} = \frac{\sigma_{s}}{1 + \epsilon_{\text{eff}}^\alpha}$$

(6)

where $\alpha$ is the Bruggeman exponent. As discussed in \cite{12}, the electrolyte volume fraction (or porosity) $\epsilon_e$ in the two electrodes is updated as

$$\epsilon_{e} = \frac{1 - \epsilon_{0, \text{add}} - \epsilon_{0, \text{active}}}{1 + \epsilon_{\text{eff}}^\alpha} = \frac{\epsilon_{0}}{1 + \epsilon_{\text{eff}}^\alpha}$$

(7)

where $\epsilon_{\text{eff}}^\alpha$ is the total mechanical strain in the SLTD, $\epsilon_{0, \text{add}}$ is the initial volume fraction of all components other than active material, e.g., binder or carbon black, $\epsilon_{0, \text{active}}$ is the initial volume fraction of the active material, and $\epsilon_{0}$ is the initial volume fraction of the electrolyte. The porosity of the separator is updated as

$$\epsilon_{s} = \frac{1 - \epsilon_{0, \text{solid}} - \epsilon_{0, \text{active}}}{1 + \epsilon_{\text{eff}}^\alpha} = \frac{\epsilon_{0}}{1 + \epsilon_{\text{eff}}^\alpha}$$

(8)

with $\epsilon_{0, \text{solid}}$ as the initial volume fraction of the solid-phase separator material. In this work, we do not consider film growth due to side reactions. However, the presented framework is capable of accounting for it. In (7) and (8), the strain field $\epsilon_{\text{eff}}^\alpha$ is computed as

$$\epsilon_{\text{eff}}^\alpha = \epsilon_{\text{elastic}}^\alpha + \epsilon_{\text{active}}^\alpha$$

with $\epsilon_{\text{elastic}}^\alpha = \frac{1}{E} \sigma_{\text{eff}}^\alpha$

(9)

where $\epsilon_{\text{elastic}}^\alpha$ and $\epsilon_{\text{active}}^\alpha$ describe the strain due to elastic deformation and Li-intercalation, respectively. In (9), $E$ is the effective Young’s modulus, whose value is different for each porous region. $\sigma_{\text{eff}}^\alpha$ is the projected stress in the SLTD computed from the thermomechanical model, which is the same for all the three porous regions. Thus, the value of $\epsilon_{\text{elastic}}^\alpha$ is different for each porous region. For the electrodes, the Li insertion/extraction induced volume change ratios are different. $\epsilon_{\text{active}}^\alpha$ is inhomogeneous in both electrodes along the SLTD due to the nonuniform Li distribution during charge/discharge. For the separator, $\epsilon_{\text{active}}^\alpha$ is zero. Thus, $\epsilon_e$ in the electrodes is location dependent and varying along the SLTD, whereas $\epsilon_e$ in the separator is homogeneous. A non-zero $\epsilon_{\text{eff}}^\alpha$ leads to an elongation or contraction of the porous composite materials and thus to a change of the distance that the charged species need to travel. This effect is reflected in the equations summarized in Table I.

Thermal coupling. The DualFoil model and the temperature field are coupled in two ways. First, the electrochemical properties, such as conductivity, diffusivity, and electrode kinetics in the equations in Table I follow an Arrhenius-type temperature dependence in the form \cite{10}

$$\mathbf{e} = \mathbf{e}_{\text{ref}} \exp \left[ \frac{E_a}{R} \left( \frac{1}{\theta_0} - \frac{1}{\theta} \right) \right]$$

(18)

where $\theta$ represents $D_s$, $D_e$, $\kappa_s$, and $\kappa_0$, and $\mathbf{e}_{\text{ref}}$ represents their corresponding reference values. Some of the electrolyte transport properties have a different dependence on temperature (see Table I). Second, the local volumetric...
heat generation rate is computed by the DualFoil model based on [6]

\[
\dot{q} = - \frac{1}{L_0} \left( \int L \sum_k a_k i_{n,k} U_{H,k} dt - IV \right), \quad \text{with} \quad U_{H,k} = -T \frac{\partial U_k}{\partial t} + U_k
\]

which accounts for irreversible heat generation due to electrochemical processes, Joule heating due to ohmic losses, and reversible entropic heat. As the heat generation rate is inhomogeneous along the SLTD, an integration over the thickness of the sandwich layer is performed in [19] to compute the heat generation rate per unit area, which is then divided by the initial thickness \(L_0\) of the sub-cell to compute the volume-averaged heat generation rate \(\dot{q}\).

### 2.3 Coupling between electrochemical and thermomechanical models

Following [14], a fine mesh with \(n_{TM}\) elements is used for the thermomechanical model, which allows us to obtain a high spatial resolution for the temperature and displacement fields. A coarse mesh with \(n_{EC}\) elements is created. Each coarse element represents a 1D electrochemical sub-cell, which spatially covers multiple thermomechanical elements, as shown in Fig. [1]. The 1D electrochemical sub-cell is discretized in the SLTD, along which the electrochemical model is solved. Note that the coarse element may be comprised of multiple and/or partial cell sandwich layers, and the 1D discretization and direction corresponds to the average of the corresponding layers. Due to the high conductivity of the current collectors, the electrical potential between two electrodes at any location of the jellyroll is approximated as identical, although the approximation introduces some error at high C rates in cells without multiple or continuous tabs [45]. Thus, the overall electrochemical behavior of the jellyroll can be modeled by connecting \(n_{EC}\) sub-cells in parallel, where all the sub-cells have an identical electrical potential, but in principle differing temperature, current density, stress level, and porosity. The governing equations are solved with a Crank-Nicolson method in the 1D setting for each sub-cell. In this framework, the \(n_{EC}\) sub-cells can be specified independently from one other. It allows us to assign different initial parameters (e.g., thickness, porosity) to each sub-cell to account for a non-uniform material distribution in the jellyroll.

A two-way coupling scheme is used to exchange information between the thermomechanical and the electrochemical submodels through volume-averaged quantities and projected stresses, as shown in Fig. [1]. Even though the electrochemical model is solved in the 1D setting, due to the complex physics and the large number of total sub-cells, the electrochemical simulation can still be expensive. In order to obtain an optimal compromise between simulation...
accuracy and runtime, we can vary the ratio between the number of thermomechanical elements and the number of electrochemical sub-cells. To obtain high resolution of the electrochemical state variables, we can define an electrochemical sub-cell mesh that aligns with the layers of the jellyroll. But often this is not necessary, as the adjacent cell sandwich layers can have similar electrochemical properties, which allows us to use one coarse electrochemical element to cover multiple cell sandwich layers to improve the computational efficiency. In addition, the presented approach also allows us to assign more sub-cells in those regions that require a higher spatial resolution of the electrochemical state variables and fewer sub-cells in those regions that tend to have more uniform states.

### 2.3.1 Averaged quantities for the mechanical field

![Figure 2: Illustration of the stress projection procedure. (a) Front view of the coarse electrochemical mesh as shown in Fig. 1 where a local coordinate system with basis vectors \( \boldsymbol{n}, \boldsymbol{s}, \boldsymbol{t} \) is defined with \( \boldsymbol{n} \) indicating the SLTD for each element, along which the mechanically coupled 1D DualFoil model is solved. (b) Coordinate system transformation between Cartesian system with basis vector of \( \boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3 \) and the local coordinate system \( \boldsymbol{n}, \boldsymbol{s}, \boldsymbol{t} \). As indicated by the red arrows, \( \boldsymbol{n} \) is changing with the jellyroll geometry. The input stress value to the electrochemical model is \( \sigma^{nn} \), which is the component value of \( \sigma \) in the \( \boldsymbol{n} \) direction. To obtain \( \sigma^{nn} \), we first calculate \( \sigma' \) in an intermediate coordinate system \( \boldsymbol{e}_1', \boldsymbol{e}_2', \boldsymbol{e}_3' \) by rotating \( \boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3 \) along \( \boldsymbol{e}_2' \) with an angle of \( \delta \). Next, \( \boldsymbol{e}_1', \boldsymbol{e}_2', \boldsymbol{e}_3' \) is rotated along \( \boldsymbol{e}_2' \) with an angle of \( \phi \) to obtain \( \sigma \) in the \( \boldsymbol{n} \) direction.](https://mc04.manuscriptcentral.com/jes-ecs)

The mechanically coupled DualFoil model takes the averaged stress \( \sigma^{nn} \) of the jellyroll in the SLTD to update the porosity in Eq. 9. \( \sigma^{nn} \) represents the stress component of the homogenized Cauchy stress tensor \( \sigma \) computed from the thermomechanical model in Section 2.1 in the direction of \( \boldsymbol{n} = E^{-T} \mathbf{N} \). \( \mathbf{N} \) is the SLTD defined in the reference configuration and \( \boldsymbol{n} \) describes the SLTD obtained in the actual configuration. As illustrated in Fig. 2, we use \( \boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3 \) to denote the basis vectors of the Cartesian coordinate system. For an arbitrary direction \( \boldsymbol{n} \), to obtain the value of \( \sigma^{nn} \), we need to first rotate \( \sigma \) along \( \boldsymbol{e}_1 \) with an angle of \( \delta \) to an intermediate coordinate system \( \boldsymbol{e}_1', \boldsymbol{e}_2', \boldsymbol{e}_3' \) with a rotation tensor \( Q_3 \) defined as

\[
Q_3 = \begin{bmatrix}
\cos(\delta) & -\sin(\delta) & 0 \\
\sin(\delta) & \cos(\delta) & 0 \\
0 & 0 & 1
\end{bmatrix}.
\] (20)

The corresponding stress tensor \( \sigma' \) expressed in the coordinate system \( \boldsymbol{e}_1', \boldsymbol{e}_2', \boldsymbol{e}_3' \) is computed as \( \sigma' = Q_3^T \sigma Q_3 \). We then rotate \( \sigma' \) along \( \boldsymbol{e}_2' \) with an angle of \( \phi \) to the local coordinate system \( \boldsymbol{n}, \boldsymbol{s}, \boldsymbol{t} \) with a rotation tensor \( Q_2 \) defined as

\[
Q_2 = \begin{bmatrix}
\cos(\phi) & 0 & \sin(\phi) \\
0 & 1 & 0 \\
-\sin(\phi) & 0 & \cos(\phi)
\end{bmatrix}.
\] (21)

The corresponding stress tensor \( \tilde{\sigma} \) expressed in the coordinate system \( \boldsymbol{n}, \boldsymbol{s}, \boldsymbol{t} \) is computed as \( \tilde{\sigma} = Q_2^T \sigma' Q_2 = Q_2^T Q_3^T \sigma Q_3 Q_2 \). Since each coarse electrochemical element is associated with multiple (assuming a ratio of \( k \)) fine thermomechanical elements, as shown in Fig. 1 the volume-averaged stress \( \sigma^{nn} \) for a specific electrochemical element is computed as

\[
\sigma^{nn} = \frac{1}{k} \sum_{i=1}^{k} \frac{1}{|B_i|} \int_{B_i} \tilde{\sigma}_{11} dV,
\] (22)

where the integration is performed via the Gaussian quadrature rule with two Gauss points being used in each direction. The same \( \sigma^{nn} \) is assigned to each node of the 1D electrochemical mesh to compute the \( e_{\text{elastic}} \) defined in 3. Interested readers are directed to Ref. [44] for details of numerical integration on Gaussian quadrature.
thermomechanical model requires $\bar{\omega}$ to compute the $F_{\text{swelling}}$ in (11), which is computed from the mechanically coupled DualFoil model as

$$\bar{\omega} = \frac{\int_{\Omega(C)} \Omega(C) l^0_{\text{active}} dl}{L_0},$$  \tag{23}$$

where $\Omega(C)$ is the average relative volume change of the active material. The integral in (23) calculates the total volume change of the sub-cell due to Li insertion and extraction.\footnote{In a 1D electrochemical sub-cell, the area of the separator is assumed to be constant. Thus, the volume change of the sub-cell is equivalent to its thickness change in the SLTD. $\bar{\omega}$ is a hypothetical thickness change that would occur assuming no external mechanical pressure on the sub-cell with incompressible electrolyte.} One can refer to \cite{12} for a more detailed description. The same $\bar{\omega}$ computed from one specific sub-cell is assigned as a Gauss point value to those thermomechanical elements that are associated with it to update the 3D stress and the displacement fields.

### 2.3.2 Averaged quantities for the thermal field

The DualFoil model takes a volume-averaged temperature $\bar{\theta}$ that is computed by the 3D thermomechanical model as an input parameter. Since each coarse electrochemical element is associated with multiple (assuming a ratio of $k$) fine thermomechanical elements, as shown in Fig. 1, the volume-averaged temperature $\bar{\theta}$ for a specific sub-cell is computed via

$$\bar{\theta} = \frac{1}{\sum_{i=1}^{k} \int_{B_i} dV} \sum_{i=1}^{k} \int_{B_i} \theta dV,$$  \tag{24}$$

where the integration is performed via the Gaussian quadrature rule with two Gauss points being used in each direction. The same $\bar{\theta}$ is assigned to each node of the 1D electrochemical sub-cell. Thus, the temperature in each sub-cell is homogeneous, whereas it can be different across the electrochemical sub-cells. For each sub-cell, a volumetric heat generation rate $\dot{q}$ is calculated based on (19). The same $\dot{q}$ is assigned as Gauss point values to those thermomechanical elements that are associated with the sub-cell to update the temperature field. This is transferred to all associated thermomechanical elements and used in the next iteration step to update the temperature field.

### 2.4 Simulation flowchart

The electrochemical model is coupled with the thermomechanical model via volume-averaged quantities, such as temperature $\theta$, heat generation rate $\dot{q}$, intercalation-induced volume change ratio $\bar{\omega}$, and mechanical stress $\sigma^{nn}$. This information is exchanged between the 3D finite element code based on deal.II and the 1D DualFoil model code through API (application programming interface).

Figure 3: Illustration of the information flow in the proposed coupled multiphysics battery simulation framework. Abbreviation: TM (thermomechanical), EC (electrochemical), API (application programming interface).
Table 2: Summary of the simulation steps in the proposed multiphysics battery simulation framework.

A. Initialize a simulation with the proper initial state variables, boundary conditions, and physical parameters.

B. Compute quantities of interest at a new time step $t$

(a) Update the thermal loading and the mechanical loading. The former consists of an external convective boundary condition and an internal heat generation rate $\dot{q}$. The latter consists of an externally applied loading and an internal intercalation-induced swelling $\bar{\omega}$.

(b) Solve the temperature and displacement fields with the finite element method.

(c) Pass the volume-averaged temperature $\bar{\theta}$ and the projected stress value $\sigma_{nn}$ to the DualFoil model via the API.

(d) Apply the electrical loading through the API. This is done indirectly by applying a guessed, uniform value of the voltage to each electrochemical sub-cell (e.g., converged voltage of the previous time step).

(i) Independently solve the electrochemical properties and states of each sub-cell with finite difference method based on the input potential $V$, temperature $\bar{\theta}$, and stress $\sigma_{nn}$.

(ii) Compute the sum of the output volumetric current densities of all the electrochemical sub-cells and check if it matches the applied volumetric current density.

(iii) If the relative error $\epsilon > \text{tol}$ with $\text{tol} = 10^{-8}$, as shown in Fig. 3, adjust the applied sub-cell voltage $V$ and repeat steps (b) and (d).

(e) Once converged, pass the volumetric quantities $\dot{q}$ and $\bar{\omega}$ from each sub-cell to its associated thermomechanical element(s) via the API.

(f) Output state variables of interest.

C. Move forward to the next time (loading) step.

D. Stop the simulation if certain criteria are met (e.g., a specified cutoff potential is reached).

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Following [46], the homogenized Young’s modulus of the jellyroll in the SLTD in Table 5 is computed based on Voigt averaging via

$$E = \left( \sum_i \frac{L_i}{L_0} \frac{1}{E_i} \right)^{-1} \quad (25)$$

where $i$ refers to the individual components in the jellyroll, e.g., the current collectors, electrodes, and the separator. $L_i$ is the thickness of each component. For the 18650 cell, the thicknesses for the anode current collector, anode, separator, cathode, and cathode current collector are 5 $\mu$m, 73 $\mu$m, 20 $\mu$m, 60 $\mu$m, and 9 $\mu$m, respectively, resulting in

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3 Model Parameterization

We apply the model to investigate how mechanical deformation affects the electrochemical behavior of an 18650 cell and a prismatic cell. Both cells consist of a graphite anode, a LiCoO$_2$ cathode, a Celgard 2400 separator, and a 1M LiPF$_6$ salt in EC/DMC electrolyte. The parameterization of the simulation model corresponding to these cells is presented in detail in previous works [12, 14] and is taken over in this study. For the cylindrical cell, the previous work [14] was carried out without accounting for mechanical deformation. Thus, we re-parameterize the cell for the mechanically coupled electrochemical model by combining reported values from the literature, measured values from experiments, and optimized values from simulations. Several of the parameters, e.g., diffusion coefficient, reaction rate, activation energy, etc., were re-tuned by numerical optimization, i.e., by minimizing the L2-norm of the difference of the original experimental voltage profile reported in [13] and the simulated voltage profile at given C-rates. The full set of material parameters used in the simulations are summarized in Tables 3 through 5.

Following [46], the homogenized Young’s modulus of the jellyroll in the SLTD in Table 5 is computed based on Voigt averaging via

$$E = \left( \sum_i \frac{L_i}{L_0} \frac{1}{E_i} \right)^{-1} \quad (25)$$

where $i$ refers to the individual components in the jellyroll, e.g., the current collectors, electrodes, and the separator. $L_i$ is the thickness of each component. For the 18650 cell, the thicknesses for the anode current collector, anode, separator, cathode, and cathode current collector are 5 $\mu$m, 73 $\mu$m, 20 $\mu$m, 60 $\mu$m, and 9 $\mu$m, respectively, resulting in

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and the invisible in-plane deformation of pouch cells observed in experiments, a very small Poisson’s ratio $\nu$ resulting in an effective Young’s modulus of 537 MPa. As discussed in [47, 48], due to the porous nature of the cell is assumed for the jellyroll.

First, we consider a brick-shape jellyroll with a size of 2.5 mm $\times$ 0.167 mm $\times$ 1.0 mm. The SLTD is parallel to the Y-axis. The jellyroll is meshed with 250 elements for the thermomechanical model, as shown in Fig. 4. Each thermomechanical element corresponds 1:1 to an electrochemical sub-cell, i.e., the fine mesh and the coarse mesh illustrated in Fig. 1 are identical with the ratio between the number of electrochemical elements and the number of thermomechanical element.

| Parameters                       | Li$_x$C$_6$ | Celgard 2400 | Li$_x$CoO$_2$ |
|----------------------------------|-------------|--------------|--------------|
| Thickness, $\mu$m                | 73          | 20           | 60           |
| Electrolyte volume fraction      | 0.238       | 0.4          | 0.17         |
| Inert filler volume fraction     | 0.06        | 0.1          | fitted       |
| Diffusion coefficient in solids, m$^2$/s | 1.33e-13 | 3.0e-13      | fitted       |
| D50 particle radius, $\mu$m      | 9.5         | 3.85         | vendor       |
| Reaction rate constant, mol/(m$^2$ $\cdot$ s) | 3.3e-8     | 1.67e-11     | fitted       |
| Density, g/cm$^3$                | 2.11        | 5.10         | [14]         |
| Theoretical specific capacity, mAh/g | 372        | 273.85       | [14]         |
| Matrix conductivity, S/m         | 10.0        | 10.0         | [14]         |
| Initial value of x and y         | 0.805       | 0.462        | fitted       |
| Solid state diffusion AE, K      | 11920       | 2633         | fitted       |
| Insertion kinetics AE, K         | 20253       | 2630         | fitted       |
| Bruggeman exponent               | 1.42        | 1.13         | 1.56         |
| Effective Young’s modulus, N/m$^2$ | 4.6e8      | 5.0e8        | 5.6e8        |

Table 3: List of parameters of electrodes and separator for the 18650 cell. AE: normalized activation energy, $E_a/R$ in Eq. (18).

| Parameter/Property                     | Value/Expression |
|----------------------------------------|------------------|
| Salt concentration (1 M LiPF$_6$ in EC/DEC), M | 1.0 |
| Conduction AE, K                        | 4000             |
| Diffusion AE, K                         | 328              |
| Conductivity, mS/cm                     | $\kappa_{\text{e,ref}} = 0.91 c_e \left[ (-10.5 + 0.072 \theta - 6.5 \times 10^{-5} \theta^2) 
+ (0.668 - 0.0172 \theta + 2.6 \times 10^{-5} \theta^2) c_e 
+ (0.494 - 8.56 \times 10^{-4} \theta) c_e^2 \right]^2 
\log_{10} \left( D_e \exp \left( \frac{1}{9 - \frac{1}{298}} \right) \right) 
= -5.08 - 0.22 c_e - \frac{\theta - 237 - 5.17 c_e}{55.87} 
$ |
| Transference number                     | $t_e = 0.399$    |
| Activity coefficient                    | $rac{d \ln f_2}{d \ln c_e} = 0.24 \cdot 0.5 - 0.982 [1.0 - 0.0052 (0.966 \theta - 294)] c_e^{1.5} $ |

Table 4: List of parameters and properties of the electrolyte in the 18650 cell[14].

Table: $^{5}$The reported Li ion diffusion coefficients in both graphite and LiCoO$_2$ vary by several orders of magnitude, with a fitting bound of [1e-15, 1e-11] m$^2$/s being identified for graphite, and a bound [1e-16, 1e-11] m$^2$/s for LiCoO$_2$. [49–58].

4 Results and discussion

4.1 Non-uniform mechanical deformation

First, we consider a brick-shape jellyroll with a size of 2.5 mm $\times$ 0.167 mm $\times$ 1.0 mm. The SLTD is parallel to the Y-axis. The jellyroll is meshed with 250 elements for the thermomechanical model, as shown in Fig. 4. Each thermomechanical element corresponds 1:1 to an electrochemical sub-cell, i.e., the fine mesh and the coarse mesh illustrated in Fig. 1 are identical with the ratio between the number of electrochemical elements and the number of
Table 5: List of parameters for the 3D homogenized thermomechanical model. The heat equation related parameters \( \rho \), \( C_p \), and \( \kappa_{\theta} \) are adopted from [14] unless otherwise noted. \(^a\): through-plane thermal conductivity, \(^b\): in-plane thermal conductivity.

| Component                  | Material    | \( E \) (N/m\(^2\)) | \( \nu \) (-) | \( \rho \) (kg/m\(^3\)) | \( C_p \), (J/(kg \cdot K)) | \( \kappa_{\theta} \), (W/(m \cdot K)) |
|---------------------------|-------------|------------------------|---------------|---------------------------|-----------------------------|------------------------------------------|
| Jellyroll (18650) Composite | Composite   | 5.46e8                 | 0.01 [47, 48] | 2708                      | 781                         | 1.5\(^a\)/28\(^b\)/28\(^b\)         |
| Jellyroll (prismatic) Composite | Composite   | 5.37e8                 | 0.01 [47, 48] | 2724 [59]                 | 920 [59]                    | 1.5\(^a\)/28\(^b\)/28\(^b\)         |
| Can, CID (18650) Steel     | Steel       | 1.9e11                 | 0.295         | 8030                      | 449                         | 16                                       |
| Gasket (18650) HDPE        | HDPE        | 6.0e8                  | 0.46          | 960                       | 2054                        | 0.4                                      |
| Tabs (18650) Nickel        | Nickel      | 2.05e11                | 0.305         | 8900                      | 411                         | 92                                       |
| Current collector Copper   | Copper      | 1.21e11                | 0.34          | -                         | -                           | -                                        |
| Aluminum                  |             | 6.9e10                 | 0.334         | 2719                      | 778                         | 202                                      |

Figure 4: Illustration of the jellyroll meshed geometry. The SLTD is parallel to the Y-axis. The same mesh is used for both the thermomechanical model and the electrochemical model.

Figure 5: Top view of the solution distribution of both SOC and current density for three simulation conditions at the end of discharge. (a) and (b) show that case (i) results in a uniform SOC and current density distribution in the jellyroll. (c-f) show that the newly proposed simulation framework is capable of capturing the spatially varying cell state quantities. The inhomogeneity of these quantities arises in (c,d) because a random initial porosity for the anode is used in the simulation. In (e,f), the inhomogeneity comes from the externally applied inhomogeneous mechanical loading.
thermomechanical elements being one. Each sub-cell is discretized into 80 intervals in the SLTD to solve for the electrochemical state variables. The material parameters listed in Table 3-5 are used. The jellyroll is galvanostatically discharged at $I = 2 \text{A}$ with a fixed homogeneous temperature at $\theta = 20^\circ \text{C}$ under three different scenarios considering material parameter variations and mechanical loading: (i) uniform material distribution without external mechanical loading, (ii) non-uniform material distribution without external mechanical loading, where the initial anode porosity of electrochemical elements has a random distribution in the range of $[0.226, 0.25]$, equivalent to a $\pm 5\%$ initial anode porosity variation, and (iii) uniform material distribution with non-uniform external mechanical loading in the SLTD that varies in a linear way along the X-axis with $\sigma_{nn} = -5 \text{MPa}$ at $X = 0$ and $\sigma_{nn} = 5 \text{MPa}$ at $X = 2.5 \text{mm}$. In all three cases, the porosity may change due to swelling and shrinkage of the active material.

The current density and SOC distribution at the end of discharge of the three cases are shown in Fig. 5. Based on the specified discharge protocol, about 45% of the cell capacity is obtained for each case, resulting in the final value of the SOC around 0.55. For case (i), because of the uniformity of both internal and external states, a uniform SOC and current density distribution in the jellyroll is observed, as shown in Fig. 5(a,b). For case (ii) and (iii), due to either the non-uniform initial cell state or non-uniform external mechanical loading, the jellyroll has unbalanced internal electrochemical states. A spatially varying SOC and current density distribution is observed for both cases, as shown in Fig. 5(c-f). These results confirm the capability of the newly proposed framework to capture spatially varying quantities in a Li-ion battery.

4.2 Simulation of a cylindrical cell

Next, an 18650 cell is discharged at 4A rate under both natural ($h = 12.5 \text{W/(m}^2\cdot\text{K})$) and forced ($h = 49.5 \text{W/(m}^2\cdot\text{K})$) convection conditions, with $h$ as the external heat transfer coefficient. The original experimental setup can be found in [14]. In the simulation, we use a fine mesh with 61,700 elements for the thermomechanical model, as shown in Fig. 7 with the jellyroll being divided into 90 sub-cells (3 in the radical direction, 6 in the azimuthal direction, and 5 in the height direction) for the electrochemical simulation (see Fig. 8).

In the simulation, the proper mechanical constraint at the interface between different parts of a battery cell is not easy to measure. In addition, the cell initial internal pressure might vary among vendors. Future experimental work is needed to determine if there is any relative movement between the jellyroll and other parts during charge/discharge, and what is the appropriate range of initial internal pressure level inside a battery cell. The presented model can
Figure 8: Illustration of the SOC and current density distribution in the coarse electrochemical sub-cells at the end of discharge under the forced convection condition. The non-uniformity of the SOC and current density is more correlated to the non-uniform temperature than the projected stress field in Fig. 7.

Figure 9: Illustration of voltage and core temperature profile of the 2.2-Ah 18650 cell for a 4A (~ 1.8C) discharge under both natural and forced convection conditions. A very good match between simulations and experiments is obtained for the voltage. The predicted core temperature differs from the measured values by less than 3°C.

be used to address these uncertainties and evaluate how different cell configurations will impact the electrochemical response of battery cells. In this simulation, we neglect the initial internal pressure applied to the jellyroll. We assume that all the parts are fully connected with no relative movement between each other during charge/discharge.

The simulated cell voltage and core temperature of the 18650 cell is compared with experimental measurements for both natural and forced convection conditions, as shown in Fig. 9. We observe that the simulated cell voltage profiles match the experimental discharge curves very well. The predicted core temperature differs from the measured values by less than 3°C. High resolution non-uniform temperature and projected stress distributions from the simulation are shown in Fig. 7(b). Because of the aforementioned assumption, a high stress is observed at the bottom of the jellyroll, as shown in Fig. 7(b), which differs from other regions primarily due to the mechanical interaction between the jellyroll and other parts. Under the forced convection condition, about 35% of the cell capacity is discharged (see Fig. 9), resulting in the final value of the SOC around 0.65. The SOC and current density distribution in the coarse electrochemical sub-cells are shown in Fig. 8 from which we can observe that, in this particular simulation, the non-uniform SOC and current density is more correlated to the non-uniform temperature than the projected stress, where the SOC is lower in the region with higher temperature due to its lower electrochemical resistance during discharge.
Figure 10: Illustration of the whole jellyroll geometry and the mesh of 1/8th of it used for the simulation.

![Diagram](image1)

Figure 11: Illustration of voltage and thickness ratio change of the prismatic jellyroll at a C/2 discharge with $\theta = 25^\circ$C. Both voltage profile and the swelling ratio have a good match with the experimental data.

![Diagram](image2)

Figure 12: Illustration of the simulation results of the prismatic cell at the end of a C/2 discharge. (a) Front view of the mesh with the dashed box indicating the zoom region. (b) Local projected stress concentration due to jellyroll geometry. (c) Non-uniform SOC distribution due to localized mechanical deformation. (d) Unbalanced current density due to localized mechanical deformation.
4.3 Simulation of a prismatic cell

Lastly, a prismatic cell, which has been previously studied and parameterized in [12,59,61], is investigated. For the sake of simplicity, we neglect the can of the battery cell and simulate only the jellyroll. In addition, because the jellyroll is symmetric with respect to \( x-\)plane, \( y-\)plane, and \( z-\)plane, only 1/8th of it is simulated, as shown in Fig. [10] 511 elements for both the thermomechanical model and the electrochemical model are used. Furthermore, as pointed out in [59], this prismatic cell has a fairly uniform temperature distribution due to a very small Biot number. To better understand the impact on the electrochemical behavior of the jellyroll from the mechanical deformation, an isothermal condition is considered. The jellyroll is discharged at the \( \text{C}/2 \) rate at a temperature of 25°C with an initial capacity of \( \sim 2.7 \text{ Ah} \). Both the voltage profile and the thickness ratio change of the prismatic cell are shown in Fig. [11] where a very good match of the voltage profile between simulation and experimental data is observed. The simulation takes the experimentally measured swelling ratio vs SOC for both graphite and \( \text{LiCoO}_2 \) active particles as inputs and outputs the averaged thickness change of the whole jellyroll. As pointed out in [12], the observed difference in the thickness ratio change arises because the swelling ratio vs SOC for both graphite and \( \text{LiCoO}_2 \) used in the simulation is measured from a different cell.

To understand how mechanical deformation affects the electrochemical behavior of this prismatic cell, the distributions of the projected stress, SOC, and current density are shown in Fig. [12]. From Fig. [12]b, one can observe that a high stress concentration rises in the simulation due to intercalation-induced volume change and the curved geometry of the jellyroll. This high stress concentration results in a non-uniform SOC and current density distribution. At the end of the discharge, a \( \sim 8.5\% \) difference is observed between the maximum and the minimum SOC values. The current density shows a \( \sim 5.8\% \) difference between the maximum and the minimum values. The unbalanced electrochemical states resulting from inhomogeneous mechanical deformation due to the jellyroll geometry may lead to non-uniform \( \text{Li-plating} \) during charging, as observed at the edge of prismatic cells [62,63]. This effect is the subject of a manuscript in preparation, in which the same model is applied to cell charging.

5 Conclusion

In this work, a coupled framework of an electro-chemo-thermo-mechanical model is proposed that is capable of efficiently and accurately simulating LIBs at the cell/pack level. A cylindrical cell and a prismatic cell are studied to demonstrate the performance of the presented framework. The simulation results obtained from this new framework reveal that localized stress concentration arises due to intercalation-induced volume change and jellyroll geometry. Such localized mechanical deformation can result in unbalanced electrochemical states that could potentially be related to non-uniform \( \text{Li-plating} \). These results demonstrate the impact of including mechanical effects in a battery simulation. However, it is worth to point it out that the quantitative results due to mechanical deformation presented in this work should only be interpreted qualitatively. Future research concerning the accurate measurement of effective mechanical properties of each component in a Li-ion battery, the understanding of how to properly impose mechanical constraints inside the cell, and the careful experimental design to thoroughly measure the electrochemical, thermal, and mechanical parameters is needed to achieve a comprehensive understanding of the coupling between the thermomechanical effects and the electrochemical behavior of LIBs. In addition, for cells operating under high external mechanical loading and/or for cells designs with larger active material volume change (e.g. Si-based), a more sophisticated coupling scheme between mechanics and electrochemistry will be needed to account for the bulk electrolyte movement.

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Nomenclature

\[ \begin{align*}
\alpha_0 & \quad \text{initial active interfacial area per unit electrode volume (specific interfacial area), } 1/\text{m}^2 \\
C_e & \quad \text{Li}^+ \text{ concentration of electrolyte in the current configuration, mol/m}^3 \\
C_s^{\text{max}} & \quad \text{maximum surface concentration in the reference configuration, mol/m}^3 \\
\bar{C} & \quad \text{volume-averaged solid-phase Li concentration in the reference configuration, mol/m}^3 \\
C_e & \quad \text{Li}^+ \text{ concentration of electrolyte in the reference configuration, mol/m}^3
\end{align*} \]
\( C_p \) • specific heat capacity, J/(kg \cdot K)
\( C_s \) • Li surface concentration of active particles in the reference configuration, mol/m\(^3\)
\( D_e \) • bulk electrolyte diffusion coefficient, m\(^2\)/s
\( D_{e, \text{eff}} \) • effective electrolyte diffusion coefficient, m\(^2\)/s
\( E \) • Young's modulus, N/m\(^2\)
\( E_a/R \) • activation energy, K
\( f^\pm \) • salt activity coefficient
\( F \) • Faraday's constant, 96485 C/mol
\( F \) • deformation gradient
\( F^{-T} \) • transpose of the inverse of deformation gradient
\( F_{\text{elastic}} \) • elastic component of deformation gradient
\( F_{\text{swelling}} \) • swelling component of deformation gradient
\( F_\theta \) • thermal expansion contribution in deformation gradient
\( i_{n,k} \) • interfacial charge transfer current density, A/m\(^2\)
\( i \) • current density for individual electrochemical element, A/m\(^3\)
\( I \) • cell-sandwich current density, A/m\(^2\)
\( I \) • volumetric current density, A/m\(^3\)
\( I_e \) • electrolyte-phase current density in the reference configuration, A/m\(^2\)
\( I_s \) • solid-phase current density in the reference configuration, A/m\(^2\)
\( J_{\text{active}} \) • averaged Jacobian of active particles
\( \bar{J} \) • Jacobian
\( \bar{J}_{\text{elastic}} \) • determinant of the elastic deformation gradient
\( J_n \) • pore-wall flux across interface in the reference configuration, mol/(m\(^2\) \cdot s)
\( k \) • subscript, refer to different reactions
\( k_0 \) • reaction rate constant, m\(^2\)/s \cdot (m/mol)^{1/2}
\( L_0 \) • total thickness of one sandwich layer, m
\( L_i \) • thickness of the individual component of a sandwich layer, m
\( n \) • direction of the sandwich layer in the spatial configuration
\( N \) • direction of the sandwich layer in the reference configuration
\( P \) • the first Piola-Kirchhoff stress, N/m\(^2\)
\( \bar{Q} \) • volume-averaged solid-phase Li concentration gradient in the reference configuration, mol/m\(^4\)
\( \dot{q} \) • volumetric rate of heat generation, W/m\(^3\)
\( Q \) • rotation tensor
\( R \) • gas constant, 8.314 J/(mol \cdot K)
\( R_0^p \) • initial radius of solid particles, \(\mu\)m
\( t^+ \) • cationic transference number
\( U \) • open-circuit potential, V
\( U_H \) • enthalpy potential, V
\( V \) • cell voltage, closed-circuit potential, V
\( W \) • elastic strain energy density, N/m\(^2\)
\( X \) • reference coordinate
\( \alpha \) • Bruggeman's exponent
\( \alpha_a \) • anodic transfer coefficient
\( \alpha_c \) • cathodic transfer coefficient
\( \epsilon_{\text{active}}^0 \) • initial volume fraction of solid active materials
\( \epsilon^0 \) • initial volume fraction of additional components
\( \epsilon_{\text{add}}^0 \) • initial volume fraction of solid phase in the electrolyte
\( \eta_s \) • surface overpotential, V
\( \varphi \) • deformation mapping
\( \kappa_\theta \) • thermal conductivity, W/(m \cdot K)
\( \kappa_e \) • bulk electrolyte conductivity, S/m
\( \kappa_s \) • bulk electronic conductivity, S/m
\( \kappa_{e,\text{eff}} \) • effective electrolyte conductivity (Li\(^+\)), S/m
\( \kappa_{s,\text{eff}} \) • effective electronic conductivity (e\(^-\)), S/m
\( \lambda \) • Lamé constant, N/m²
\( \mu \) • Lamé constant, N/m²
\( \nu \) • Poisson’s ratio [-]
\( \bar{\omega} \) • volume change ratio
\( \phi_e \) • electrolyte potential, V
\( \phi_s \) • solid-phase potential, V
\( \rho \) • density, g/m³
\( \sigma_{nm} \) • projected stress in SLTD, N/m²
\( \sigma \) • the Cauchy stress tensor, N/m²
\( \bar{\theta} \) • volume-averaged temperature, K
\( \theta \) • temperature, K
\( \theta_0 \) • reference temperature, K
\( I \) • second order identity tensor

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