



A novel phenomenological multi-physics model of Li-ion battery cells



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HIGHLIGHTS

- A novel multi-physics model of Li-ion batteries on the cell-level is developed.
- The proposed model couples electric, thermal, and mechanical behaviors of the cell.
- The model predicts surface temperature, SOC, and force at pack conditions.
- Intensive experimental validations confirm that the model has high accuracy.

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ABSTRACT

A novel phenomenological multi-physics model of Lithium-ion battery cells is developed for control and state estimation purposes. The model can capture electrical, thermal, and mechanical behaviors of battery cells under constrained conditions, e.g., battery pack conditions. Specifically, the proposed model predicts the core and surface temperatures and reaction force induced from the volume change of battery cells because of electrochemically- and thermally-induced swelling. Moreover, the model incorporates the influences of changes in preload and ambient temperature on the force considering severe environmental conditions electrified vehicles face. Intensive experimental validation demonstrates that the proposed multi-physics model accurately predicts the surface temperature and reaction force for a wide operational range of preload and ambient temperature. This high fidelity model can be useful for more accurate and robust state of charge estimation considering the complex dynamic behaviors of the battery cell. Furthermore, the inherent simplicity of the mechanical measurements offers distinct advantages to improve the existing power and thermal management strategies for battery management.

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1. Introduction

Rechargeable Li-ion batteries (LIBs) have various advantages compared to alternative batteries. LIBs not only provide high power/energy density over a broad temperature range of operation, but also exhibit no memory effect, low self-discharge ratio, and long cycle life [1–4]. These advantages make LIBs an ideal candidate for a wide variety of applications from small-scale portable electronics to massive-scale energy storage systems.

However, problems that persist in existing LIBs limit their application in transportation, military, and aerospace due to the stringent safety standards. The limitations of current battery technology include underutilization, capacity fade, thermal

runaway, and stress-induced material damage. In order to overcome these challenges, understanding the complex multi-physics beyond the LIBs is indispensable.

The significant efforts have been devoted to identify the complex physics behind the LIB which would be useful to predict operational states, and thereby enhances operational safety and enlarges operational window. The porous electrode theory, which solves Lithium diffusion dynamics and charge transfer kinetics in a paired intercalation electrode system, has been proposed to predict the electrical response of a cell [6]. This physics-based model can predict microscopic behavior and performance, whereas it requires a large computational power to solve the differential equations. An equivalent circuit model has also been proposed for control-oriented purposes to estimate the electrical response and the amount of heat generation [7–9]. A variety of heat transfer models have been created and validated through experiments [10–13]. Several lumped parametric thermal models have also been

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proposed for control-oriented purposes with advanced power management schemes [14–16]. Numerical simulations on the cell-level and pack-level with computational fluid dynamics and finite element methods have been conducted to predict the thermodynamics of Li-ion battery cells and packs with experimental validation [17–20]. Coupled models between electrochemistry and heat transfer have also been suggested to elucidate the coupled effect of the current, potential, and temperature on the state of charge (SOC) and state of health (SOH) for large-scale LIBs [21–24].

Recent research focuses more on the structural response. The volume change of electrode materials in LIBs under charge process has been intensively investigated to characterize the electrochemical-induced stress and strain [25–32]. The effects of prestress and stress-evolution on capacity fade over time or cycling have also been studied [33,34]. This research promotes theoretical and experimental understanding of the structural response of the LIBs, especially in microscopic perspective. Moreover, the macroscopic stress and strain responses from two sources, i.e. Li-ion intercalation and temperature variation, is observable and measurable with the advancement of sensor technology, suggesting that the structural response can become a sensitive gauge for characterizing the battery state [5,35]. However, studies related to stress and strain on the cell-level are still few, especially in modeling perspective. Moreover, the coupled model of stress and strain with electrochemical reaction and thermodynamics of the LIBs has not been investigated in great detail, even though this fully-coupled multi-physics model can improve the safety and reliability of batteries, enhance the capability of cells and packs, and eventually prolong the lifetime of the LIBs.

This paper proposes a fully-coupled phenomenological multi-physics model of the LIBs for the first time. The proposed multi-physics model couples the electric, thermal, and swelling effect on the force in pack conditions. The important parameters, which govern the thermal characteristics and mechanical responses on the cell-level, were estimated from experimental data. The main purpose of this phenomenological model is to predict the temperature and force induced from the volume change of battery cells, which is driven by prestress, Li-ion intercalation, and temperature variation, in pack conditions. Experimental validation at a variety of operational conditions confirms that the proposed multi-physics model accurately predicts the temperature and the compression force during operation at the overall SOC regions for a wide range of temperature and preload conditions.

2. Experiments

This study used a flat-wound type prismatic 5 Ah Li-ion cell obtained from a Ford Fusion HEV battery pack. Detailed information of the Li-ion cell is available in Ref. [5].

Three LIBs were sandwiched together between two Garolite end-plates and bolted to maintain a constant compression length to replicate conditions experienced in a battery pack. The battery cells were separated by spacers that maintain compression between the cells while allowing for airflow between them for cooling purposes (Fig. 1). Battery temperature was measured on the surface of the cell by using resistance temperature detector sensors (RTDs). Battery force was measured by using four load cells, Omega LC8150-250-100 sensors with a 450 N full-scale range and an accuracy of 2 N, placed on the corners of the fixture. The fixture was placed in a thermal chamber for ambient temperature control, and the force and temperature data were collected via an 18-bit data acquisition card and a National Instruments module. Bitrode model FTV was used for battery cycling.

Several experiments were performed to characterize and validate parameters used in the multi-physics model and are outlined below.

In the first experimental sets, the quasi-static force was measured at several different ambient temperature and two different preload conditions. Prior to discharge, the battery was fully charged using a CCCV protocol [35] at 5 A (1.0 C) and rested 3 h at a fixed ambient temperature of 25 °C as regulated by the thermal chamber; the voltage was clamped after reaching 4.1 V, at which time it was held until the current tapered to C/100 (50 mA). Then, the temperature of the thermal chamber was changed to the desired temperature (−5 °C, 10 °C, 45 °C). Each temperature variation was followed by 3 h of rest time to ensure thermal equilibrium. This procedure was omitted to measure the quasi-static force at the ambient temperature of 25 °C. In order to obtain the desired SOC ranging from 0% to 100% with 5% interval, the battery was discharged with a 0.4 C current of actual capacity with an appropriate time (7.5 min). The actual capacity was calculated by using coulomb counting method during discharge with 0.4C rate from 4.1 V to 3.0 V herein. Each discharge was followed by 3 h of rest time to ensure the quasi-static equilibrium. This procedure was repeated four times with the identical preload, 670 N at 0.05 SOC, but different four ambient temperature (−5 °C, 10 °C, 25 °C, 45 °C) during discharge. These four experiments were also repeated again with different preload, i.e. 450 N at 0.05 SOC.

In the second experimental sets, three pulse excitation experiments were performed for validating the estimated coefficient of thermal expansion at an ambient temperature of 25 °C and the wide range of preload conditions. The battery was fully charged using standard CCCV protocol prior to discharge. Then, the battery was discharged with a 2 A (0.4 C) current for appropriate time to obtain three desired SOC. In the first experiment, a 50 A charge sustaining pulse with a 1 s period (0.5 s charge and 0.5 s discharge) was applied for 2.5 h at 0.48 SOC. The initial preload was set to 1276 N. In the second experiment, a 50 A charge sustaining pulse with a 100-s period (50 s charge and 50 s discharge) was applied for 2.5 h at 0.22 SOC with an initial preload of 145 N. The final experiment consisted of a 50 A charge sustaining pulse with a 100-s period (50 s charge and 50 s discharge). The pulse was applied at 0.74 SOC with an initial preload of 330 N.

In the final experimental sets, intensive experimental validation was performed for the proposed multi-physics model with the US06 duty cycle at a variety of operational conditions (Table 1). A current profile measured from a Ford Fusion hybrid over US06 driving cycle was applied in experimental sets.

Three additional fixtures (Fig. 1) were prepared to collect the second and third experimental sets. Acquiring one set of data (shown as symbols in Fig. 4(a) and (b)) takes one week in the first experimental setup. In total, the first experimental setup required two months to collect the data shown in Fig. 4. Therefore, conducting experiments in parallel with four fixtures significantly reduced the time needed to gather the experimental data. Moreover, obtaining data with different cells has allowed us to guarantee that the proposed model is adequate for simulating the behavior of different cells. Additional details on the applicability of the model are discussed in Section 4.4.

3. Model description

The multi-physics model consists of three major components (Fig. 2): a coupled Electro-Thermal Model (ETM), swelling models, and a force estimator. The ETM estimates the state of charge (SOC) and the surface/core temperature of the battery cell with the measured current and ambient temperature. The swelling models calculate the total amount of swelling for the battery cell at unconstrained conditions with SOC and the surface/core/ambient temperatures provided by the ETM. The force estimator calculates the reaction force caused by the volume change of the battery cell

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