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Computational design and refinement of self-heating lithium ion batteries

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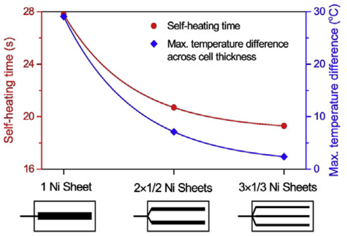
HIGHLIGHTS

- We present & validate the first model for a new class of self-heating Li-ion batteries.
- Non-uniform temperature and current distributions in a SHLB are predicted.
- Internal temperature gradient greatly affects self-heating time & energy consumption.
- Multi-sheet design with optimized self-heating time & energy consumption is proposed.

GRAPHICAL ABSTRACT



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ABSTRACT

The recently discovered self-heating lithium ion battery has shown rapid self-heating from subzero temperatures and superior power thereafter, delivering a practical solution to poor battery performance at low temperatures. Here, we describe and validate an electrochemical-thermal coupled model developed specifically for computational design and improvement of the self-heating Li-ion battery (SHLB) where nickel foils are embedded in its structure. Predicting internal cell characteristics, such as current, temperature and Li-concentration distributions, the model is used to discover key design factors affecting the time and energy needed for self-heating and to explore advanced cell designs with the highest self-heating efficiency. It is found that ohmic heat generated in the nickel foil accounts for the majority of internal heat generation, resulting in a large internal temperature gradient from the nickel foil toward the outer cell surface. The large through-plane temperature gradient leads to highly non-uniform current distribution, and more importantly, is found to be the decisive factor affecting the heating time and energy consumption. A multi-sheet cell design is thus proposed and demonstrated to substantially minimize the temperature gradient, achieving 30% more rapid self-heating with 27% less energy consumption than those reported in the literature.

1. Introduction

Lithium ion batteries suffer from severe performance loss at low temperatures [1–4], limiting their use in many applications like electric vehicles (EVs). The driving range of EV per charge, 105 miles at 75 °F (23.9 °C) as reported by American Automobile Association [5], drops by 57% to 43 miles at 20 °F (−6.7 °C), exacerbating driving range anxiety which is already a major barrier to mainstream adoption of EVs. Fundamental reasons for poor battery performance at low temperatures include high viscosity of the electrolyte

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and hence low Li^+ diffusivity, low ionic conductivity of the electrolyte, high solid-electrolyte interphase (SEI) layer impedance, and high interfacial kinetic resistances, especially in the graphite anode.

Much work has been conducted in the past decade to improve the performance of Li-ion batteries at subzero temperatures [6–12]. One prevalent approach is to search for additives that can improve electrolyte performance at low temperatures [10,13]. Most of these electrolyte additives, however, also deteriorate cell performance and cycle life at high temperatures. Another approach is to preheat the battery to an optimal temperature before use [14–16]. Ji and Wang [16] thoroughly reviewed a wide range of heating strategies, although most have such issues as low heating efficiency, long heating time and high energy consumption.

Most recently, we experimentally discovered a novel battery structure, the self-heating Li-ion battery (SHLB) [3], which can rapidly self-heat from −30 °C to 0 °C in less than 30 s and thereafter bring about a 10-fold power boost over state-of-art Li-ion batteries, with only ~5.5% of cell energy consumed. Fig. 1a illustrates the structure of an SHLB. Aside from the three main components of a conventional Li-ion cell: an anode, a cathode and an electrolyte/separator, the SHLB inserts a thin nickel (Ni) foil, coated with electrically insulating polymer and sandwiched between two single-sided anode layers, into the center of the SHLB. One end of the Ni foil is connected to the negative terminal, welded together with tabs of all anode layers. The other end of the Ni foil extends outside the cell to form a third terminal, the activation terminal. A switch is used to connect the activation terminal with the negative terminal. The working principle of the SHLB can be explained via the electrical circuit diagram in Fig. 1b. At temperatures lower than 0 °C, the switch is left open to force current flow through the Ni foil, generating substantial ohmic heat that rapidly warms up the battery materials and electrochemical interfaces. Once the cell temperature reaches or exceeds 0 °C, the switch is closed such that the current bypasses the Ni foil and the cell acts as a conventional cell, working in the optimal temperature range with superior performance.

Here, for the first time, we describe an electrochemical-thermal (ECT) coupled model developed to seek a fundamental understanding of the self-heating process (hereafter referred to as activation) and to discover key design factors affecting the time and energy needed for self-heating. Furthermore, we shall unravel a major advance in the SHLB technology through computer simulations.

2. Electrochemical-thermal coupled model

The SHLB pouch cell contains a number of multiple anode and cathode layers with separators in between, along with a thin nickel foil for self-heating stacked in the middle of the cell, as illustrated in Fig. 1a. Each anode or cathode layer is composed of a current-collecting foil with active materials coated on both sides. Given the stacking structure, the pouch cell can be considered as multiple cell units connected in parallel, each composed of one anode layer, one cathode layer, and two separators, as illustrated in Fig. 1a. Fig. S1 in the electronic supplementary information (ESI) depicts the current flow among the various cell units as well as the Ni foil in the activation process of the SHLB. All cell units share the same voltage, but we shall note that the current of each unit may be quite different if their local states such as temperature and state of charge (SOC), differ.

A generic electrochemical-thermal (ECT) modeling framework based on three-grid method of Luo and Wang [17] and Kalupson et al. [18] is adopted here. In it the thermal model is solved on a macro-scale grid discretizing a multi-layer, large-format cell (displayed in Fig. 1c, where each mesh corresponds to one cell unit defined in Fig. 1a). Each cell unit is further discretized into a set of meso-grids in the thickness direction (Fig. 1d), on which the electrochemical processes are simulated. In addition, the solid-state diffusion is numerically solved on the micro-grid dividing active material particles into a number of finite elements (Fig. 1d). These model components are briefly summarized in the following.

2.1. Electrochemical model

The electrochemical model for each cell unit of anode/electrolyte-separator/cathode contains the following conservation equations:

Charge conservation in solid electrodes:

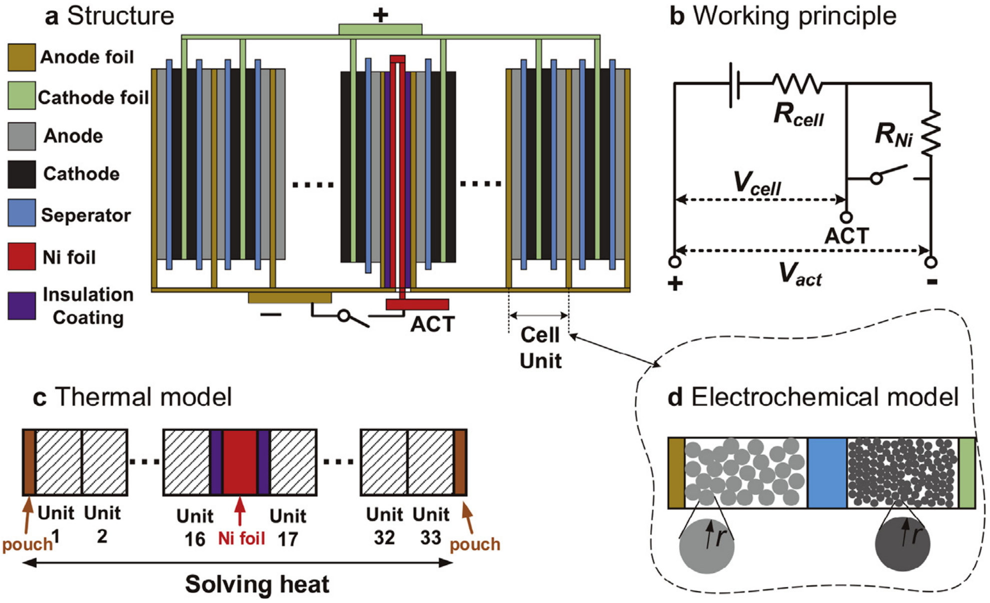

Fig. 1. (a) Structure of a self-heating Li-ion battery (SHLB) and illustration of the multi-layer pouch cell. (b) Electrical circuit diagram showing the working principle of the SHLB and definition of cell voltage (V_{cell}) and activation voltage (V_{act}). (c) Sketch of the thermal model. (d) Sketch of the electrochemical model corresponding to one cell unit.