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Thermal analysis of Lithium-ion cell: Measurements and Modeling

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ABSTRACT

Lithium-ion (Li-ion) cells are widely used in electrochemical energy storage systems due to their advantages, such as lightweight, high-energy density, and ability to recharge. However, Lithium-ion cells still have the risk of a hazard named "Thermal runaway", which can lead to fire and explosion. Thermal control is crucial to keep the cell safe and healthy and prevent "aging" acceleration. An intensive study was devoted to the thermal management of battery cells. For this application, knowing cell temperature is a critical issue since the temperature can be measured only on the cell's surface.

In the present research the thermal response of Li-ion cells was studied theoretically and experimentally. A mechanistic numerical model was developed to simulate the electrochemical and thermal transport phenomena in the cell. The model can calculate the cell temperature in any point and time during charge or discharge operation mode.

In the experimental part of the present study, a novel measurement method is being developed using optic fibers with FBG sensors to investigate the internal temperature behavior of Lithium-ion. This approach provides us with the opportunity to get a highly accurate temperature map of Lithium-ion cells under different loads and consequently to get more experimental data for improving existing analytical models.

Keywords: Lithium-ion (Li-ion) cells, Elecrto-Chemical Thermal analysis

מוטיבציה: פילוג טמפרטורה בתא- בקרה

מדידה, מודל

1. Introduction

Lithium-ion cells have significantly contributed to remarkable advances in science and industry, especially in the electric vehicle revolution and the global transition to renewable energy sources to achieve a net-zero carbon emissions future [Tamilselvi, 2021; Chombo, 2020]. However, due to such rapid developing progress there are still a lot of uncovered issues and shortage of scientific knowledge and experimental data. Researchers and industry stakeholders address these challenges by investigating various aspects, from battery component chemistry, mining of raw materials, to batteries assembling, Battery Management System (BMS), optimization and safety issues.

Temperature control is one of the critical factors in the operation of Li-ion cells, as it directly impacts both safety and performance. The cell temperature is determined by heat generation during operation and heat dissipation from the cell surface. The heat transfer intensity depends on cell geometry and cooling system performance, while internal heat conduction is affected by the thermal properties of the cell [Drake, 2015]. A safe operating temperature range for Li-ion cells, typically from minus 20°C to 60°C during discharge and from 0°C to 45°C during charging, varies depending on cell chemistry [Ortega, 2021; Zhang, 2022]. Excessive temperatures can lead to "thermal runaway," making it essential to maintain an optimal thermal environment while also understanding and mitigating internal triggers that initiate and accelerate this hazardous process.

Predicting the thermal behavior of lithium-ion batteries during operation and keeping the battery within safety temperature range relies on the Battery Thermal Management System (BTMS), an integral part of the Battery Management System (BMS). An effective BTMS control depends on robust mathematical models; however, these models are typically built on general thermophysical concepts and surface temperature data of cells. To enhance model accuracy, it is crucial to expand experimental datasets and deepen the study of lithium-ion batteries' internal thermal characteristics.

A step forward in battery thermal management field is the experimental study of temperature distribution inside Lithium-ion cell. Fiber Bragg Grating (FBG) techniques rely on the reflection of light at specific wavelengths within an optical fiber, which shifts in response to temperature or strain changes. Study of the thermal behavior of lithium-ion cells using optical fibers with FBG sensors can significantly contribute to the advancement of future battery technologies.

The current research combines experimental and modeling efforts to expand knowledge in the field of battery thermal management systems. The experimental part involves investigating the internal temperature distribution of lithium-ion cells under operation (charge-discharge test circles). This part is devoted to proving hypotheses about the possibility of getting precision data of temperature distribution within Lithium-ion cells without significant effects on the primary cell properties. For that reason, five (5) regular samples of the Lithium-ion cells and five of the same cell type samples with embedded optic fibers with FBG-sensors will be manufactured and tested. Results of the sample charge-discharge tests will be presented later.

The modeling part aimed to study the Lithium-ion battery simulation approaches and ways of improving existing analytical models. N "in house" mechanistic model combined with COMSOL Multiphysics® software were used as a main tool for creating “white box” Electro-Chemical Thermal Model of the Lithium-ion cell. The properties of the components of Lithium -ion cell is usually a confidential information, for that reason data for the electro-chemical model was taken from the literature [Smith, 2007; and others].

2. Lithium-ion cell model

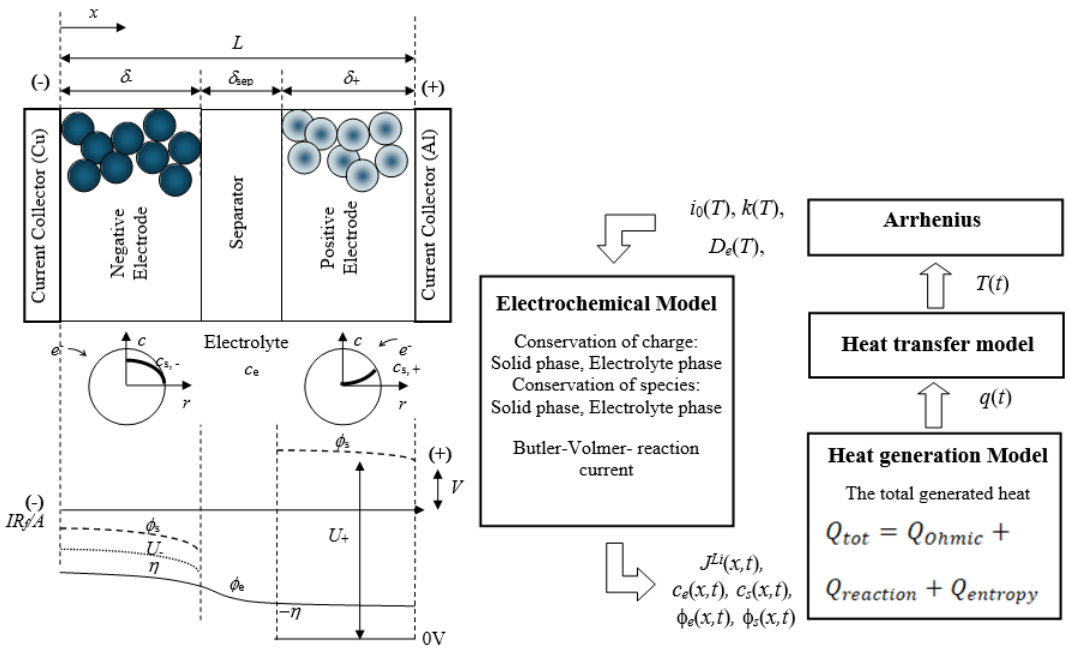
In the theoretical part a mechanistic 2D - axisymmetric model was developed

2.1. Description of the electro-chemical thermal model

2D axisymmetric Electro-chemical thermal model of cylindrical Lithium-ion cell with air convection cooling system was developed. A 1D cell sub-model was created to model the electro-chemical processes inside Lithium-ion cell and coupled with 2D axisymmetric thermal sub-model. The two sub-models were coupled by the generated heat source obtained from electro-chemical sub-model and the average temperature inside the cell from the thermal sub-model.

2.2. Governing equations

The 1D cell electro-chemical model consists of the following three domains as presented in Figure 1a: negative porous electrode, separator, and positive porous electrode. 1D model is based on the works of Newman and others [Thomas, 2002; Doyle, 1993; Baker, 2012]. Ohm's law is used to describe the charge transport in the electrodes. For electrolyte, concentrated electrolyte theory for a quiescent aprotic (1:1) electrolyte is used to describe charge and mass transport in the electrolyte phase [COMSOL User's Guide].



a) b)

Figure 1. a) the cell structure and the potential profile; b) structure of the electro-chemical thermal model of Lithium-ion cell

Electro-chemical processes in Lithium-ion cell are described by following Governing equations:

a. Conservation of charge in the electrolyte phase
b. Conservation of charge in the solid phase
c. Conservation equation of species in the electrolyte phase
d. Conservation equation of species in the solid phase

The Butler-Volmer equation is involved in the model for describing the reaction rate, j^{Li}, for Lithium-ion intercalation and deintercalation on the electrode/electrolyte interface.

The 2D Thermal model is based on General heat balance equation, which can be defined by following expressions:

Accumulated heat = Generated heat – Dissipated heat to the ambient

$$mc_p \frac{dT}{dt} = q_{tot} - hA_s(T - T_\infty) \tag{1}$$

where the heat source term

$$q_{tot} = q_{Ohmic} + q_{reaction} + q_{entropy} \tag{2}$$

$$q_{total} = I(V_{oc} - V_{load}) + IT\frac{\partial V_{oc}}{\partial T} \tag{3}$$

where

h is the coefficient of heat dissipation to the ambient [W/(m^2·K)],

A_s is the cell external surface area [m^2],

T_∞ is an ambient temperature [K],

T is a temperature of the cell [K],

c_p is a specific heat capacity of the cell [J/(kg·K)],

q_{tot} is total heat generated inside the cell [W], was obtained from 1D electro-chemical model with scaling according to the geometry of the cell.

t is a time [s],

m is a mass of the cell [kg],

V_{OC} is open circuit voltage of Lithium-ion cell [V],

V_{load} is voltage of Lithium-ion cell under load [V].

3. Experimental study

In the experimental part a novel temperature measurement method is being developed to find the temperature distribution history within the cell. For this purpose, special cells were produced with imbedded temperature sensors.

3.1. Temperature measurement consideration

Lithium-ion cell production and the chemical environment within the cell restrict the selection of temperature sensors. The following limitations were encountered:

1) High-temperature tolerance: Sensors must withstand the high temperatures that can occur during cell assembly and onset of thermal runaway (up to 300 - 800°C, depends on the experimental program).

2) Corrosion resistance: The sensors need to be resistant to the aggressive chemical environment inside the cell, including exposure to the electrolyte.

3) Compact size: Sensors must be miniature to fit into the limited space within the battery and minimize the impact on cell performance.

4) Compatibility with battery materials: Sensor materials should be chemically inert and non-reactive with battery components, including electrodes, separator, and electrolyte materials, to prevent degradation of both sensor and battery performance.

5) Safety: Sensors must be non-conductive to prevent the risk of short circuits.

6) Long-term reliability: Sensors must endure constant heating and cooling cycles during battery charging and discharging.

Temperature sensors such as thermo-resistive devices and thermocouples have significant disadvantages:

1) they require insulation to prevent electrical contact with internal components,

2) their geometry size can influence to cell operation parameters

Fiber Bragg Grating (FBG) techniques are based on the principle of light reflection at specific wavelengths within an optical fiber, which shifts in response to changes in temperature or strain. This shift allows precise measurement of internal temperature and pressure variations in real-time, making FBG sensors ideal for monitoring critical parameters in lithium-ion batteries. FBG techniques provide us with the opportunity to embed several FBG sensors along the cell by using one thin optic fiber. Based on the above, the current study has become possible with the development of novel FBG techniques.

3.2. The Samples production

Samples are produced based on commercial 1550 cylindrical Lithium-ion cells with support of Tadiran Batteries Ltd. and Bar Ilan University. Due to difficulties connected with hermitization of the cell pack, pouch pack is performed instead of solid aluminum can. In figure 4 the scheme of assembling Lithium-ion cell samples is presented. Three optical fibers are positioned at three points along the radius of the cell, placed between the electrodes and aligned along the width of electrode. Each fiber has 9 (nine) FBG-sensors with step 5 mm between them. In figure 5 the production process is presented.

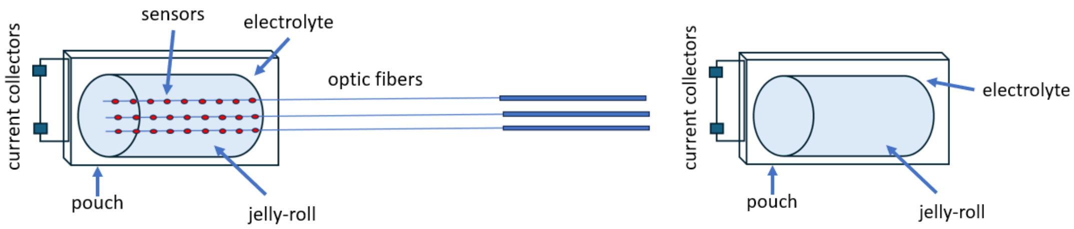


Figure 1: the scheme of assembling Lithium-ion cell sample (reference sample without thermal sensors and sample with embedded 3 optic fibers along width of the electrodes roll in 3 points of roll radius)

Figure 2. Cylindrical roll of electrodes and separator with embedded optic fibers between layers

3.3. Experimental Set-up

The experimental system is based on TEXIO controlled charging/discharging system and electrical (I -current and V-voltage) and thermal measurements. Experimental data is collected and recorded with Keysight Data Acquisition Device DAQ970A. The experimental system allows to conduct of Lithium-ion cells and battery tests and collect experimental data in a wide range of electro-thermal charge/discharge modes, including constant current (CC), constant voltage (CV), and sequence waveform or pulse current load modes.

Charge/discharge circles of the Lithium-ion cells will be conducted under different conditions: discharge C-rate from 0.5 C up to 3C with keeping cell in the climate chamber to be sure that environment temperature is constant.

Thermal measurement includes environment temperature, cell surface temperature, inner cell temperature. Thermocouple Type K is used for measuring environmental temperature close to the cell. Inner temperature is measured with FBG – sensors embedded in the cell. The FiSpec X400 Interrogator is used for generating light waves, performing onboard analysis, and recording real-time measurements, allowing for the streaming of wavelength, strain, and temperature data.

Surface temperature is measured with both types of the sensors Thermocouple Type K and optic fiber with FBG-sensors for reason to compare experimental data obtained with different type of sensors.

Detailed description of conducting experimental part of the research and experimental results will be presented at the next conference.

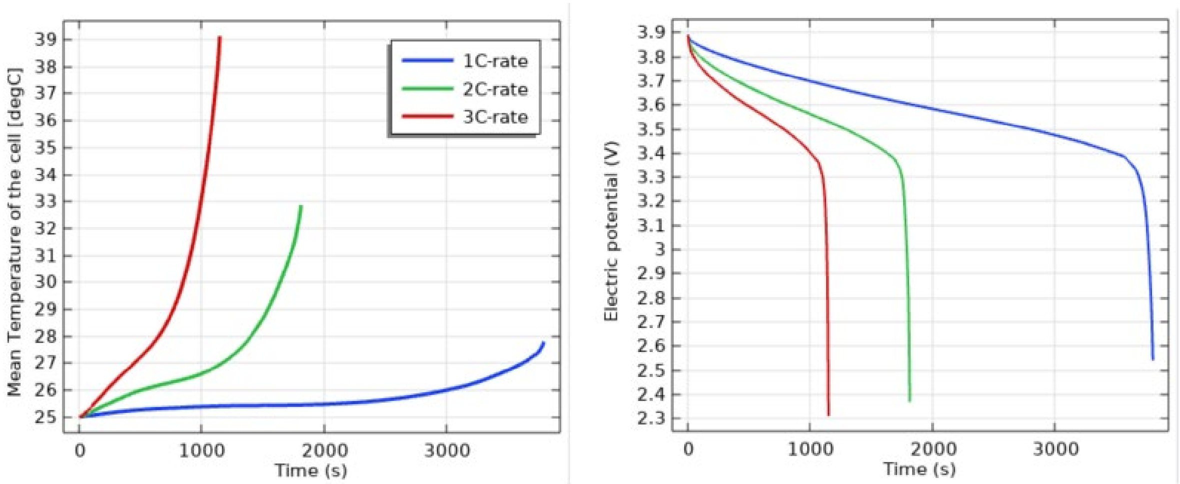
4. Results

At the current stage of the study, model predictions, the production of cells with embedded temperature sensors, and the experimental setup have been prepared for the initial calibration of the measurement system.

4.1. Results of the electro-chemical thermal model

The model was tested under various charge and discharge regimes and electro-chemical parameters has good agreement with model presented in Smith and others [Smith, 2007] paper.

Temperature distribution inside the cell and variation of mean cell temperature during Constant Current (CC) discharge tests are presented in Figure 2 and Figure 3.



a) b)

Figure 3: a) Mean temperature distribution during CC discharge tests under different load; b) Lithium-ion cell voltage drop during CC discharge tests under different load.

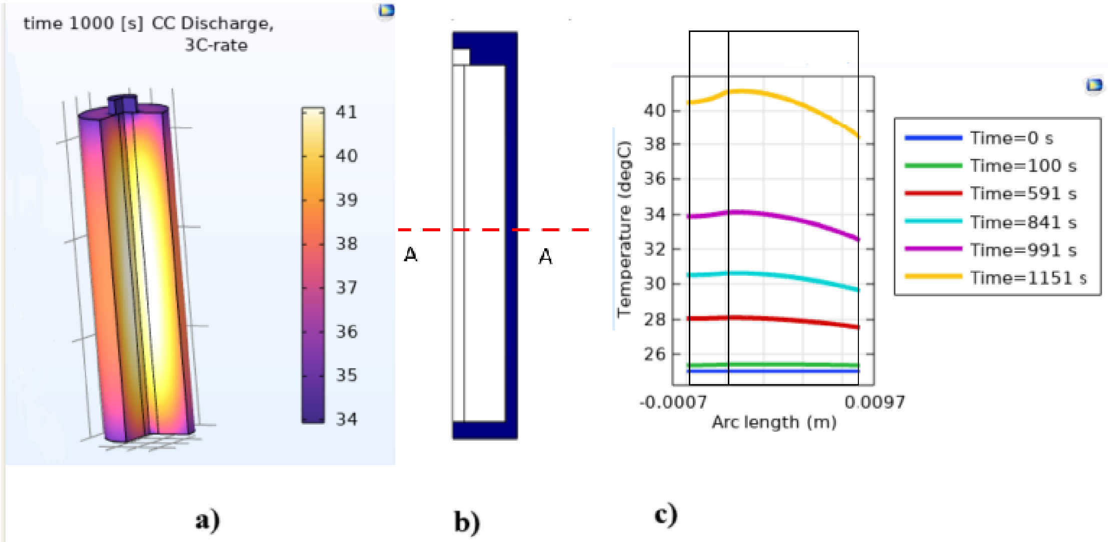


Figure 4: Cell temperature distribution under 3C-rate CC load.
a) at time point 1000 [s]; b) A-A cross section; c) temperature distribution at A-A cross section at various time point during CC discharge test.

In the future, the presented model will be improved in the course of research work using the obtained experimental data.

5. Summary

The significance of the current research arises from the safety, performance and efficiency issues in Lithium-ion cells. There are many scenarios such as mechanical damage, chemical issues inside the cell, outside thermal exploitation conditions, overcharging or over-discharging of the cell, which can lead to the cell "Thermal runaway" phenomena and as consequence fire hazards. Understanding the thermal behavior helps in the design of safer battery systems and the improve of appropriate thermal management strategies to prevent such incidents.

The temperature distribution and the heat generation in the lithium-ion cell affects the performance of cells. Higher temperatures can accelerate aging and degrade the cell's capacity, cycle life, and power capability. By investigating thermal behavior, the operating conditions can be optimized, and the overall performance and longevity of the battery can be improved.

Researching the thermal behavior of Lithium-ion batteries and utilizing optic FBG sensors can contribute to the development of future battery technologies. A step forward in this field is the experimental study of internal temperature distribution, which brings advancements in precision of mathematical models for BMS.

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