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MULTISENSORY MICROSYSTEM SIMULATION FOR EARLY DETECTION AND PREVENTION OF THERMAL RUNAWAY IN Li-Ion BATTERIES

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Abstract: This article presents the concept and modeling results of a multisensory system designed to prevent thermal runaway in lithium-ion batteries, specifically for LCO, NMC, and NCO types. The system integrates gas, temperature, and pressure sensors on a single crystal, ensuring enhanced reliability and safety by minimizing the risks of fire, explosion, or damage to battery packs. The proposed multisensory system holds significant application potential across various portable devices, including smartphones, tablets, trimmers, and different types of electric vehicles.

Keywords: simulation, thermal runaway, lithium-ion batteries, multisensory system.

I. INTRODUCTION

Lithium-ion batteries (Li-ion or LIBs) have become a ubiquitous power source in various electronic devices due to their high energy density and long service life. However, the occurrence of overheating in these batteries poses a significant safety threat, as it can lead to catastrophic failures such as fires and explosions. The process in which the temperature of the battery increases rapidly, which leads to a chain reaction of increased heat generation, is called thermal runaway (TR). Over the past decade, the issue of TR in lithium-ion batteries has garnered significant attention from both manufacturers and consumers. The processes occurring in a lithium-ion battery that lead to thermal runaway are conventionally divided into 12 stages [1]. They include dissolution of metal ions, decomposition of the SEI (Solid Electrolyte Interphase) film, reaction between lithium and electrolyte, melting of the separator, and combustion of the electrolyte. These stages are accompanied by significant changes in temperature and voltage, illustrating the complex and dangerous progression of thermal runaway.

To protect lithium-ion batteries, there is a Battery Management System (BMS), but such protection is not always effective. Thermocouples used in it to monitor temperature detect a malfunction after at least one cell has entered a state of thermal runaway, which can lead to irreversible processes [2]. An increase in temperature in the battery block leads to gas release and an increase in internal pressure in the battery. To prevent thermal runaway in a lithium-ion battery by detecting its onset at early stages, we propose a design of a multi-sensor system consisting of a gas, temperature and pressure sensor. This paper presents the results of modeling such a multi-sensor system, which can become an effective early warning option for a dangerous terminal runaway.

II. DESIGN OF MULTISENSORY MICROSYSTEM

a. Gas sensor constructions

At temperatures ranging from 70-120°C in a lithium-ion battery, the electrolyte initially starts evaporating, while the salt inside begins decomposing. These changes set off chemical reactions between the decomposed salt and either the solvent or the solid electrolyte interphase (SEI), which plays a crucial role in maintaining battery stability. Such chemical reactions cause accumulation of gases inside the battery and raise internal pressure. This gas buildup leads to an initial venting process and eventually triggers thermal runaway. This venting serves as a safety measure to release the excess pressure that has built up inside the battery. Detecting hydrogen within a lithium-ion battery cell has been highlighted by researchers as the most effective early warning sign for ensuring the safety of LIBs [3]. The concentration of hydrogen gas released during first venting varied from zero to approximately 1000 ppm [4].

Lithium-ion batteries are highly sensitive to temperature variations; therefore, it is imperative for the gas sensor to function without a heater. For the multisensory system, a metal oxide gas sensor was selected due to several advantages it offers, such as high sensitivity, rapid response time, and cost-effectiveness. Although hydrogen is the target gas, it is worth noting that metal oxide gas sensors typically lack high selectivity. However, in this case, this lack of high selectivity is advantageous because the sensor will promptly react to a range of gases that could arise during a thermal runaway event, with hydrogen being the main target.

A multi-sensor system consisting of a gas, temperature and pressure sensor was made on an anodic alumina (AA) substrate with overall dimensions of 4 × 4 × 0.43 mm^3 (Fig. 1). Interdigitated electrodes of gas sensor, consisting of three pairs of electrodes 100 µm long, 30 µm wide and with a gap of 15 µm between them. Gas-sensitive layer of ZnO-GaO with a thickness of 1 µm is located on top of the electrodes. The use of AA in modern sensors allows significant reduction in the energy consumption of thin film chemical sensors [5].

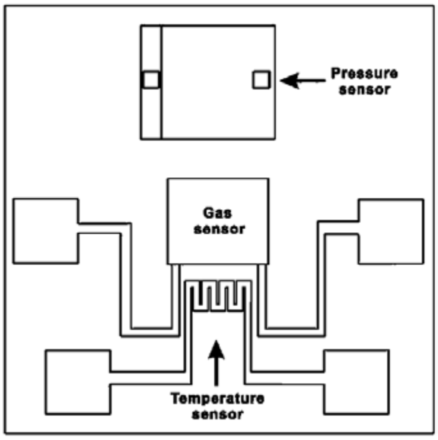


Figure 1. Design of multisensory microsystem

b. Pressure sensor constructions

The pressure inside a lithium-ion battery before and during a thermal runaway can be vary, depending on the specific conditions and the design of the battery. For cylindrical batteries, the pressure at the first venting begins to rise to 10-36 bar (1-3.6 MPa), while normal operation pressure is approximately 0.97 bar (97 kPa). Pouch batteries have the thinnest outer shell among the three types of batteries. Therefore, the pressure at the first venting in batch batteries is usually the lowest, approximately 190 kPa when first venting arise. The most common MEMS pressure sensors are piezoresistive, capacitive and resonator sensors. Advantages of a capacitive sensor: high sensitivity to pressure; less temperature sensitivity; less floor power consumption; low costs, easy to manufacture.

The proposed capacitive pressure sensor includes a lower plate of aluminum (625x530 µm, 2 µm thick), a dielectric (air and silicon nitride supporting the sides) between the plates, an upper membrane of polycrystalline silicon (530x530 µm, 12 µm), and contact pads on the membrane and bottom plate (75x75 µm) made of aluminum. The layer sizes proposed here are optimal and most effective in terms of modeling results. This design of the pressure sensor allows to accurately measuring pressure by analyzing changes in the capacity caused by the deflection of the membrane under the influence of external influences.

c. Temperature sensor design

In this work, we suggested to use a platinum wire as a temperature sensor. Such a non-contact temperature sensor based on platinum resistance thermometers avoids the problem of emissivity error. The platinum temperature sensor in our system is a four-loop platinum meander structure with a thickness of 0.3 µm. It is located directly beneath the gas sensor in the system, as shown in Figure 1. The total area of the sensor, including its contacts, is 0.55682 mm^2.

The platinum meander-based temperature sensor operates on the principle of measuring the change in electrical resistance of a platinum element as the temperature varies.

The technological process of creating such a microsystem comprising three sensors will involve four stages: 1) substrate formation (the formation of an AA substrate is described in more detail in our previous article [5]); 2) formation of the platinum temperature sensor and platinum counter-pin electrodes for the gas sensor; 3) deposition of the gas-sensitive layer on the counter-pin electrodes for the final formation of the gas sensor; 4) formation of the pressure sensor (which will include several operations for layer formation of the capacitive pressure sensor and electrodes).

III. SIMULATION RESULTS OF MULTISENSORY MICROSYSTEM

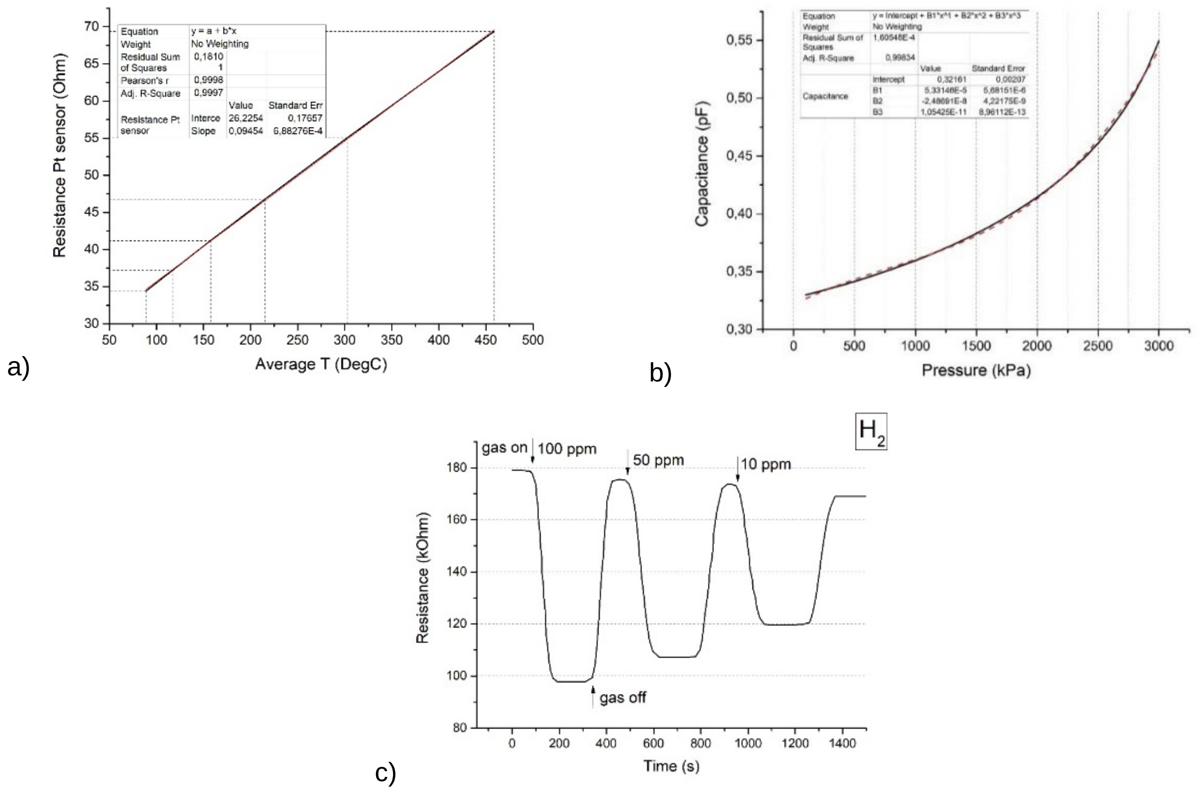
a. Sensors simulation

The process of modeling a multisensory system took place in Comsol Multiphysics 6.1 using the finite element method. The list of modules, used and their description are given in the table 1. Parameters of materials such as Young's modulus, thermal conductivity coefficient, relative permittivity, electrical conductivity and material density during modeling were taken from the libraries of materials.

Table 1. The list of modules used in Comsol Multiphysics 6.1

Type of sensor	The Comsol module	Description
Temperature sensor	Electric Currents	Creating electrical boundary conditions of a conductor with electrodes
	Heat Transfer in Solids	Simulation of heat transfer in a sensor
Pressure sensor	Solid Mechanics	Simulation of deformation of the sensor membrane under external pressure
	Electrostatics	Changing the sensor capacity during deformation
Gas sensor	Laminar Flow	Simulation of the gas flow in the system with the laminar flow regime
	Transport of Diluted Species	Modeling the transport of dilute components, with the diffusion of gases in the system
	Reaction Engineering	Initiation of chemical reactions on the surface of the gas sensor

The temperature sensor was simulated by applying a direct current to one of the electrodes. To prevent self-heating of the platinum wire, a low current of 20 μA was utilized. With increasing temperature, the sensor's resistance demonstrated a linear progression (as illustrated in Fig. 2,a). Specifically, at a temperature of 100 °C, the resistance was 35.7 Ohms, while at 200 °C, the resistance increased to 45.35 Ohms. The OriginLab program's linear approximation unveiled the relationship between resistance (R) and temperature (T), delineated by the expression R = 26.224 + 0.09454T. Thus, using this expression, it is possible to calculate the temperature from the resistance of the sensor.



a)

b)

c)

Figure 2. Sensor modeling results: a) – The dependence of Pt sensor resistance on temperature; b – The dependence of capacity on pressure; c – Correlation between gas sensor resistance and hydrogen concentration

The simulations unveiled that with rising pressure, the membrane's deformation and corresponding capacitance both escalate. Figure 2b graphically represents the correlation between capacitance and applied pressure. As previously noted, under normal operating conditions, the pressure inside the cylindric Li-ion battery is 97 kPa, at this pressure, the sensor capacity was 0.329 pF, when gases begin to be released inside the battery, the pressure inside the battery can rise to 3 MPa. At a pressure of 1 MPa, the capacity was 0.360 pF, at a pressure of 2 MPa, the capacity was 0.415 pF, at a pressure of 2 MPa, the capacity was 0.550 pF.

The polynomial approximation of the OriginLab described the relationship between the sensor capacity and the pressure value as expressions:

$$P = 0.3216 + 5.33 \times 10^{-5} C - 2{,}494 \times 10^{-8} C^2 + 1{,}054 \times 10^{-11} C^3$$

For gas sensor modeling in the Comsol, a gas reactor with periodic hydrogen supply at a concentration of ppm from 10, 50 and 100 was created during the time-dependent study. The correction coefficients based on experimental data [6] where used due to the fact that in the Comsol Multiphysics program, the task of describing all chemical reactions on the surface of the gas-sensitive layer is complicated. The change in resistance of the ZnO-GaO gas sensor based on simulation results and is presented in the figure 2,c. The sensitivity of the gas sensor for 100 ppm is determined by the expression below:

$$\frac{Rair}{gas} = \frac{179.88\ kOhm}{95.68\ kOhm} = 1.88$$

For hydrogen concentrations of 50 and 10, the sensitivity of the sensor was 1.66 and 1.47, respectively.

b. Concept application and prospects

We propose to determine three modes of battery operation: normal, dangerous and critical using the sensors described in this work (Table 1).

1. Normal safety range. In this range, the battery capacity is within normal operating limit, which depends on the packaging shape of the lithium ion battery. The temperature according to the sensor is within 20℃-50℃, which avoids overheating or hypothermia. The gas concentration level remains at zero or a safe level, without reaching critical levels that could lead to fire or explosion.

2. Dangerous Range: The battery temperature begins to approach dangerous levels (51℃-80℃) where overheating or hypothermia may occur, posing a threat to the safety and stability of the battery. Gas concentration levels may begin to increase, indicating possible problems within the battery, such as overheating or problems that could be a precursor to a fire. In this range, battery capacity may be at the edge of acceptable limits, which may indicate that measures must be taken to prevent deep discharge or overcharging, which can negatively affect the life cycle of the battery.

3. Critical Range. The battery reaches a critical level of discharge or overcharge that may result in structural damage or poor performance. The battery temperature (above 80℃) is outside the safe range, which may cause fire or explosion. The gas concentration reaches critical levels, indicating serious problems within the battery and increasing the risk of fire or explosion. For instance, the table 2 shows possible modes as an example for 18650 li-ion battery.

Table 2. Possible operation modes for 18650 li-ion battery

	Temperature, ℃	Pressure, kPa	Gas concentration, ppm
Normal safety	20-50	100	0
Dangerous	51-80	200	20
Critical	above 80	600	500

IV. CONCLUSIONS

The results of modeling a complex multisensory system including gas, pressure and temperature sensors are presented. Additionally, we delved into the operational concepts across three modes. The design of the developed multi-sensor system promises to bolster the reliability and safety of various lithium-ion battery types like LCO, NMC, and NCO by mitigating risks associated with fire, explosions, or battery pack damage. This proposed system has a wide array of potential applications, spanning from portable gadgets like smartphones, tablets, laptops, and power tools to modules in electric vehicles.

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МОДЕЛИРОВАНИЕ МУЛЬТИСЕНСОРНОЙ МИКРОСИСТЕМЫ ДЛЯ РАННЕГО ОБНАРУЖЕНИЯ И ПРЕДОТВРАЩЕНИЯ ТЕПЛОВОГО РАЗГОНА В ЛИТИЙ-ИОННЫХ АККУМУЛЯТОРАХ

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Аннотация: В данной статье представлена концепция работы и результаты моделирования мультисенсорной системы, предназначенной для предотвращения теплового разгона в литий-ионных аккумуляторах. Система объединяет датчики газа, температуры и давления на одном кристалле, обеспечивая повышенную надежность и безопасность за счет минимизации рисков возгорания, взрыва или повреждения аккумуляторных батарей. Предлагаемая мультисенсорная система имеет значительный потенциал применения на различных портативных устройствах, включая смартфоны, планшеты, триммеры и различные типы электромобилей.

Ключевые слова: моделирование, тепловой разгон, литий-ионные аккумуляторы, мультисенсорная система.