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PROACTIVE MULTISENSORY SOLUTION FOR MITIGATING THERMAL RUNAWAY RISKS IN LI-ION BATTERIES

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Abstract. The paper presents the concept and modeling results of a multisensor system designed to prevent thermal runaway in lithium-ion batteries. This is especially true for LCO, NMC and NCO batteries. The system integrates three types of sensors: a capacitive pressure sensor, a gas sensor based on a metal oxide semiconductor, and a platinum temperature sensor. Moreover, all sensors are located on a single chip, which ensures increased reliability and safety, minimizing the risks of fire, explosion, or damage to batteries. Three battery operating modes are proposed: normal, hazardous, and critical. In the normal mode, the temperature and gas concentration remain at safe levels, while in the hazardous mode, they begin to increase, indicating the possible onset of destructive reactions. In the critical mode, the battery reaches hazardous levels, which can lead to damage, fire, or explosion. The multisensor system was modeled using the COMSOL Multiphysics 6.1 package using the finite element method. This approach helps to improve the safety of lithium-ion batteries by solving the problems of monitoring their condition. The scalability of the system makes it suitable for applications in both portable electronics and electric vehicles.

Keywords: simulation, thermal runaway, lithium-ion batteries, multisensory system, gas sensor, pressure sensor, temperature sensor.

Conflict of interests. The authors declare no conflict of interests.

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ПРОАКТИВНОЕ МУЛЬТИСЕНСОРНОЕ РЕШЕНИЕ ДЛЯ СНИЖЕНИЯ РИСКА ПЕРЕГРЕВА ЛИТИЙ-ИОННЫХ АККУМУЛЯТОРОВ

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Аннотация. В статье представлены концепция и результаты моделирования мультисенсорной системы, разработанной для предотвращения теплового разгона в литий-ионных аккумуляторах. Особенно это актуально для батарей LCO, NMC и NCO. Система интегрирует три типа датчиков: емкостной датчик давления, газовый датчик на основе металлооксидного полупроводника и платиновый датчик температуры. Причем все датчики располагаются на одном чипе, что обеспечивает повышенную надежность и безопасность, минимизируя риски возгорания, взрыва или повреждения аккумуляторов. Предложены три режима работы аккумулятора: нормальный, опасный и критический. В нормальном режиме температура и концентрация газа остаются на безопасных уровнях, в опасном они начинают повышаться, что указывает на возможное начало разрушительных реакций. В критическом режиме аккумулятор достигает опасных уровней – это может привести к повреждению, возгоранию или взрыву. Мультисенсорную систему моделировали с использованием пакета COMSOL Multiphysics 6.1 с применением метода конечных элементов. Этот подход способствует повышению безопасности литий-ионных аккумуляторов, решая проблемы контроля за их состоянием. Масштабируемость системы делает ее подходящей для применения как в портативной электронике, так и для электрических транспортных средств.

Ключевые слова: моделирование, тепловой разгон, литий-ионные аккумуляторы, мультисенсорная система, газовый сенсор, датчик давления, датчик температуры.

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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 LIBs has garnered significant attention from both manufacturers and consumers. The processes occurring in a lithium-ion battery that lead to TR 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 TR.

To protect lithium-ion batteries, a Battery Management System (BMS) is used, but such protection is not always effective. Periodic fire incidents, in portable devices and electric vehicles, demonstrate that modern BMS systems sometimes fail to provide long-term protection, highlighting the urgent need for effective solutions to address this issue. For instance, the authors in [2] demonstrated that the thermocouples employed in BMS for temperature monitoring detect a malfunction only after at least one cell has already entered a state of TR, which can lead to irreversible processes.

It is well known that an increase in temperature within a battery leads to gas release, which in turn causes an increase in internal pressure [3]. To prevent TR 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.

Design of multisensory microsystem

Gas sensor constructions

At temperatures between 70 and 120 °C in a lithium-ion battery, the electrolyte begins to evaporate, and the salt inside starts to decompose. This decomposition triggers chemical reactions between the decomposed salt and either the solvent or the SEI. These reactions result in the accumulation of gases within the battery, causing the internal pressure to rise. As the pressure increases, the battery undergoes an initial venting process, which serves as a safety mechanism to release the excess pressure. However, if the temperature continues to rise after venting, it can lead to TR, where the chemical reactions inside the battery become uncontrollable. Among all the gases released within a lithium-ion battery cell, hydrogen has been identified by researchers as the most effective early warning sign for ensuring the safety of LIBs [4]. The concentration of hydrogen gas released during the first venting event can range from zero to approximately 1000 ppm [5].

LIBs 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, including 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 TR 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 4.00×4.00×0.43 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].

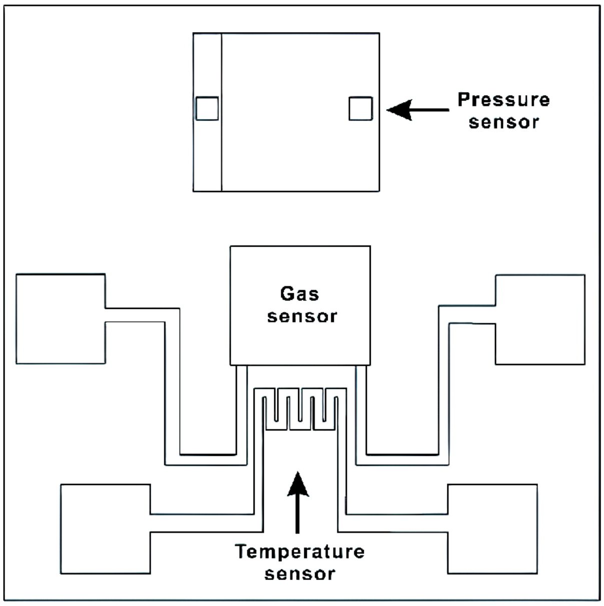

Fig. 1. Design of multisensory microsystem

Pressure sensor constructions

The pressure inside a LIBs before and during a TR 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 (1.0–3.6 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 during the first venting in pouch-type batteries is usually the lowest, approximately 190 kPa. 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 an aluminum lower plate (625×530 μm, 2 μm thick), a dielectric (air and silicon nitride supporting the sides) between the plates, an upper membrane of polycrystalline silicon (530×530 μm, 12 μm), and contact pads on the membrane and bottom plate (75×75 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.

Temperature sensor

In the study, a platinum wire was used as a temperature sensor. A contactless temperature sensor based on platinum resistance thermometers allows avoiding the error in measuring emissivity. The platinum temperature sensor in the system under consideration is a four-circuit platinum meander structure with a thickness of 0.3 μm. It is located directly under the gas sensor in the system, as shown in Fig. 1. The total area of the sensor, including its contacts, is 0.55682 mm^2. The temperature sensor based on a platinum meander operates on the principle of measuring the change in electrical resistance of a platinum element with a change in temperature.

The technological process for creating such a microsystem of three sensors includes four stages:

1) forming a substrate (the formation of a substrate from AA is described in more detail in [6]);

2) forming a platinum temperature sensor and platinum counter-pin electrodes for the gas sensor;

3) applying a gas-sensitive layer to the counter-pin electrodes for the final formation of the gas sensor;

4) formation of the pressure sensor (includes several operations for the formation of layers of the capacitive pressure sensor and electrodes).

The process of modeling a multisensory system took place in COMSOL Multiphysics 6.1 using the finite element method [7]. The list of modules, used and their description are given in the Tab. 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	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

Research results and their discussion

The temperature sensor was simulated by applying a direct current to one of the electrodes. To prevent self-heating of the platinum wire, the low current of 20 µA was utilized. With increasing temperature, the sensor's resistance demonstrated a linear progression (Fig. 2, *a*). Specifically, at the 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:

$$R = 26.224 + 0.09454T. \tag{1}$$

Thus, using this expression, it is possible to calculate the temperature from the resistance of the sensor. For gas sensor modeling in the COMSOL, a gas reactor with periodic hydrogen supply at the concentration of ppm from 10, 50 and 100 was created during the time-dependent study. The correction coefficients based on experimental data [8] 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 Fig. 2, *b*. The sensitivity of the gas sensor for 100 ppm is determined by the expression

$$\frac{R_{air}}{R_{gas}} = \frac{179.88 \text{ kOhm}}{95.68 \text{ kOhm}} = 1.88. \tag{2}$$

For hydrogen concentrations of 50 and 10, the sensitivity of the sensor was 1.66 and 1.47, respectively. For pressure sensor the simulations unveiled that with rising pressure, the membrane's deformation and corresponding capacitance both escalate (Fig. 2, *c*, *d*). As previously noted, under normal operating conditions, the pressure inside the cylindric LIBs 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 the pressure of 1 MPa, the capacity was 0.360 pF, at the pressure of 2 MPa, the capacity was 0.415 pF, at the pressure of 3 MPa, the capacity was 0.550 pF.

The polynomial approximation of the OriginLab described the relationship between the sensor capacity *C* and the pressure value *P* as expression

$$P = 0.3216 + 5.33 \cdot 10^{-5} C - 2.494 \cdot 10^{-8} C^2 + 1.054 \cdot 10^{-11} C^3. \tag{3}$$

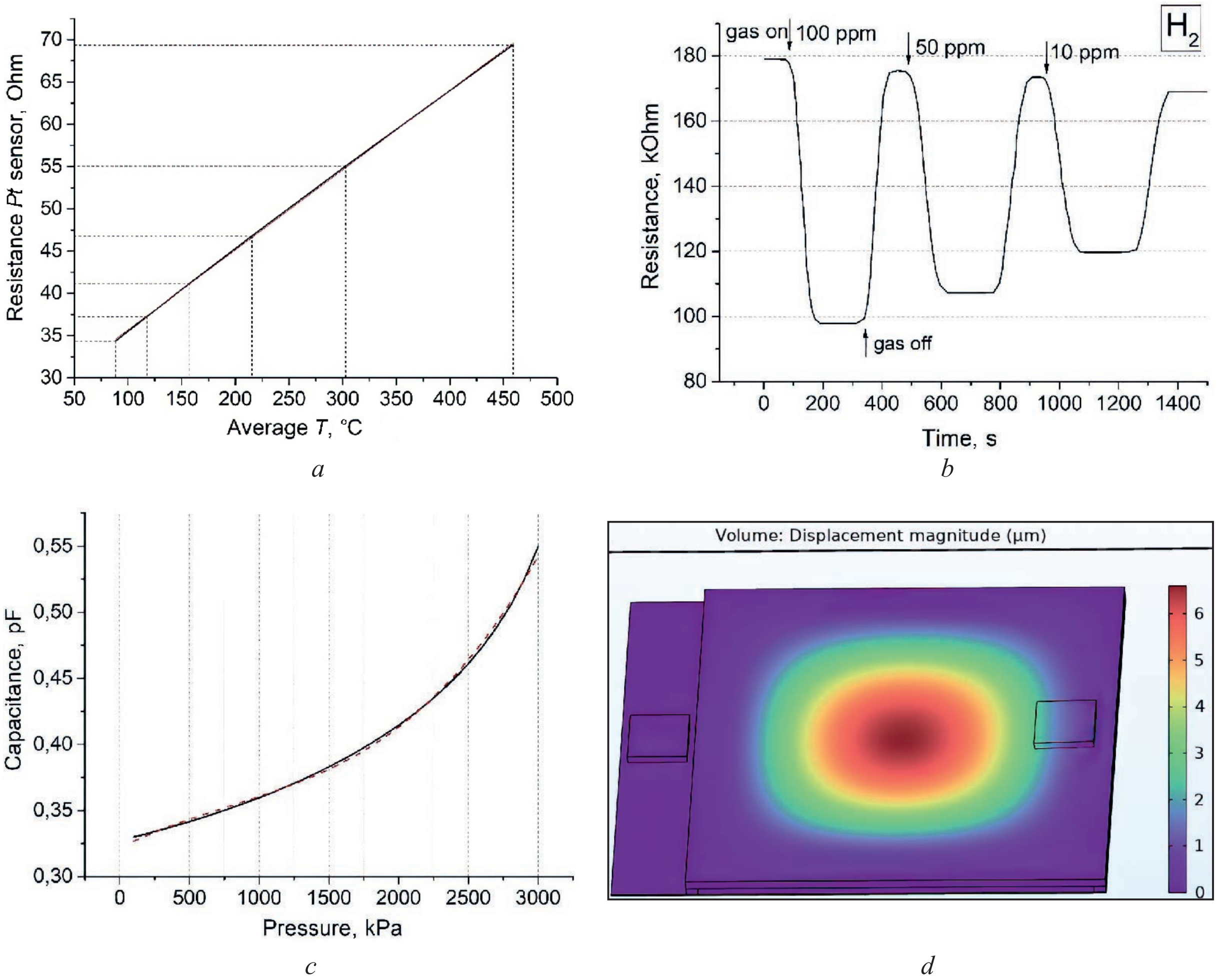

Fig. 2. Sensor modeling results: *a* is dependence of *Pt* sensor resistance on temperature; *b* is correlation between gas sensor resistance and hydrogen concentration; *c* is dependence of capacity on pressure; *d* is membrane displacement magnitude in COMSOL Multiphysics 6.1

Concept application and prospects

It is proposed to use the described sensors (to determine three operating modes of the battery: normal, dangerous and critical (Tab. 2).

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

Operation modes	Temperature, °C	Pressure, kPa	Gas concentration, ppm
Normal safety	20–60	100	0
Dangerous	61–80	200	20
Critical	Above 80	600	500

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 20–60 °C, 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 (61–80 °C) 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 °C) 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 Tab. 2 shows possible modes as an example for 18650 li-ion battery.

Sensor locations

There are two options for the location of the multi-sensory system.

1. Consider the devices with only one or several li-ion elements such as a smartphone, tablet laptops, power tools and shaving trimmers, the most promising design solution is to place the sensor near the positive electrode at the top of the batteries with cylindric and prismatic shapes (for LCO, NCA and NCM types of batteries). During the first gas release in a cylindrical lithium-ion battery, the breakdown typically occurs in the upper part of the casing, where the safety valve is located. Prismatic lithium-ion batteries also have a protective gas release mechanism to reduce pressure, similar to cylindrical batteries. This mechanism is usually implemented using a safety valve or a bursting diaphragm (often in prismatic batteries there are several in different places of the case), which open or burst when a certain internal pressure is reached, allowing gases to escape and preventing the battery from bursting. This location will provide the ability to continuously and accurately monitor the parameters, which significantly reduces the risk of unexpected incidents such as overheating or fire.

2. For electric vehicles with hundreds or even thousands (for example Tesla S) li-ion element placing a multi-sensor system should be inside a battery module (more important for NMC, NCA, then LFP battery types). We propose to allocate a specific number of cells within a module that will be monitored by a single multi-sensor system. For instance, 16 cylindrical cells (arranged in a 4×4 configuration) will be controlled by one multi-sensor system. Upon detection of any issues, the individual matrix of cells will be disconnected from the power supply. This arrangement will ensure constant monitoring of temperature, pressure and gas concentrations inside the battery pack. However, with this arrangement, the efficiency of the pressure sensor is significantly reduced, because the pressure change in the module is much lower than the pressure change inside a single lithium-ion cell. Therefore, in the case of such an arrangement, it is proposed to remove the pressure sensor from the system, and control should be carried out using a gas and temperature sensor. Or install pressure sensors on the housings of individual elements if this makes sense.

Based on the results of the study, the concept, design and simulation of a multi-sensor system for preventing TR in lithium-ion batteries are proposed. Future developments are planned to integrate an IC block for collecting, storing and transmitting data, and conduct experimental testing.

Conclusion

1. The results of modeling the complex multisensory system including gas, pressure and temperature sensors are presented. Additionally, we delved into the operational concepts across three modes and location options. 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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Authors' contribution

Fiadosenka U. S., Chenxi Yue completed the research work.
Linxi Dong, Gorokh G. G. formulated the scientific task and reviewed the article material.

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