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COMPUTER-AIDED DESIGN OF THERMOELECTRIC MICROCALORIMETRIC SENSORS

The paper deals with the design and development of thermoelectric microcalorimetric sensors for use in low-power reaction chambers. The physical and mathematical aspects of the sensitivity and response speed of sensors made of Bi-Te semiconductor material and copper-constantan-based metal legs with appropriate geometric arrangements of the legs are investigated. The paper presents a computer design algorithm, depicted as a block diagram, and also demonstrates the development of a program for automating the design process with subsequent implementation of the software. Practical examples of the development and analysis of the calculated parameters for two types of sensors are presented to identify their advantages in measuring low thermal powers and fast processes, respectively.

Key words: microcalorimetry, thermoelectric microcalorimetric sensors, computer-aided design of sensors, software.

Introduction

The measurement and control of microscopic thermal powers in such fields as microcalorimetry, biochemistry, pharmacy and technological research occupy an important place in the development of new technologies and products [1 – 3]. In this context, the accuracy and sensitivity of thermoelectric sensors play a key role in monitoring and controlling processes in the reaction chambers of microcalorimeters [4 – 12]. The development of such sensors requires innovative approaches to material selection, calculation of geometric parameters, and integration with software to automate the design process and optimize their performance.

Existing challenges include not only the selection of optimal materials and structures, but also the need to develop software that automates the processes of calculation and study of sensor characteristics. This will ensure higher accuracy and operational efficiency at minimal thermal powers, and can also accelerate the process of adaptation to specific conditions of use. The need for the development of microcalorimetric sensors is very relevant for industries where microscopic temperature changes can have significant consequences for the quality and safety of products [13 – 24].

The purpose of this work is to develop software for automating the process of computer-aided design of highly sensitive thermoelectric microcalorimetric sensors. This, in turn, will improve the functionality of such sensors by implementing advanced algorithms and computer simulation, which will ensure significant progress in the accuracy of measurements and the response speed of such devices.

1. The task of designing thermoelectric sensors for microcalorimeters

To formulate the problem of designing thermoelectric sensors for microcalorimeters, we will consider their operation in isothermal microcalorimeters.

In general, an isothermal microcalorimeter is shown in Fig. 1.

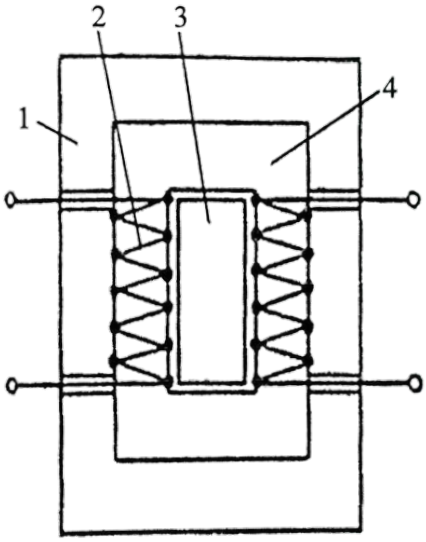


Fig. 1. Isothermal microcalorimeter: 1 – thermostatic block; 2 – sensor; 3 – reaction chamber; 4 – medium between thermostatic block and reaction chamber.

The objects under study are placed in the reaction chamber 3. To avoid heat exchange with the environment, a thermostatic block 1 is used. Measuring sensors 2 are placed between the reaction chamber and the thermostatic block.

The thermal conductivity of medium 4 between the reaction chamber and the thermostat must be sufficiently high. Then the heat does not accumulate in the microcalorimeter, but passes to the thermostatic block and is dissipated in it. The temperature difference between the reaction chamber and the thermostat is very small.

As stated above, thermoelectric sensors are an excellent tool for measuring heat flows. We will consider thermoelectric metal and semiconductor sensors with star-shaped and radial arrangement of thermocouple legs.

The operation of thermoelectric sensors is characterized by their main parameters, in particular: sensitivity, response speed, sensor resistance, number of thermocouple legs in the sensor.

When designing thermoelectric sensors, it is important to determine the sensitivity and response speed. For example, if during microcalorimetric measurements thermal processes in the reaction chamber occur quickly, it is important that the response speed of the microcalorimetric sensors be high. In the case where small thermal powers are released in the reaction chamber, highly sensitive sensors are required.

Let us establish the dependence of the sensitivity and response speed of thermoelectric sensors on the physical parameters and dimensions of the materials they are made of.

The sensitivity of a thermoelectric sensor is determined by the formula:

$$\gamma = \frac{\alpha}{\chi} \cdot \frac{L}{S} \tag{1}$$

The response speed is characterized by a time constant which is determined as:

$$\tau = \frac{c}{\chi} \cdot \frac{L}{S} \cdot \frac{1}{n} \quad (2)$$

where α is the Seebeck coefficient; χ is the thermal conductivity; c is the thermal conductivity and heat capacity of the thermoelement legs, respectively; *n* is the number of thermoelement legs; *L, S* are the length and cross-sectional area of the thermoelement leg.

As is known, metals the thermocouple sensors are made of have a thermal conductivity greater than that of semiconductors. Therefore, as can be seen from formula (1), a thermoelectric semiconductor sensor is highly sensitive compared to a metal one, provided that the geometric dimensions of their legs are equal.

But the ratio c/χ in metals is much smaller than in semiconductors, therefore, from formula (2) it is clear that with equal geometric dimensions of the legs of metal and semiconductor sensors, the response speed of metal sensors is greater than that of semiconductor ones.

From the above-established dependence of sensitivity and response speed on the physical properties of materials, it follows that for microcalorimetric measurements of thermal processes with increased response speed, metal thermoelectric sensors should be used, and when measuring thermal processes with the release of reduced thermal power, semiconductor sensors should be used.

Highly sensitive semiconductor sensors may have a response speed lower than that required for some fast thermal process in the reaction chamber. In contrast, metal sensors with a high response speed do not detect processes with low thermal power release.

In addition to the physical properties of the materials the thermoelectric sensors are made of, the geometric dimensions of the thermocouple legs also affect their sensitivity and response speed. From formulae (1) and (2) it follows that the length of the thermocouple legs *L* affects the sensitivity and response speed. As *L* increases, the sensitivity of the sensors increases, but the response speed decreases.

This dependence leads to the question: what should be the length of the thermocouple legs in order for the parameters of the thermoelectric sensor to be optimal?

An important parameter of a thermoelectric sensor is its resistance. To coordinate the operation of microcalorimetric sensors with electrical measuring devices included in their electrical circuit, it is necessary to select a sensor resistance close to the resistance of the measuring device.

Thus, the task of designing thermoelectric sensors for microcalorimeters is reduced to finding the optimal values of the following parameters:

- the number of thermocouple legs in the thermopile design,
- sensor resistance,
- the length of thermoelement legs whereby the values of thermoelectric sensor parameters will be optimal.

To solve this problem, first of all, it is necessary to specify the operating range of measuring powers in the reaction chamber. Depending on this range, the design of the thermoelectric sensor can be selected.

For this sensor design, the following parameters must be set:

- height of the microcalorimeter reaction chamber;
- diameter of the microcalorimeter reaction chamber;
- cross-sectional area of the thermoelement leg;
- geometry of the arrangement of legs (distance or angle between thermoelement legs);
- distance between thermopiles;
- physical properties of the material the legs are made of;
- thermoEMF value;

- heat capacity
- thermal conductivity;
- electric conductivity,

as well as equations relating this data to the parameters of thermoelectric sensors.

Knowing the height and diameter of the reaction chamber, as well as the geometric dimensions of the thermocouple legs and their location, it is possible to determine the density of the legs around the reaction chamber (packing density).

Since the sensor resistance includes the resistances of all thermoelement legs, it is necessary to know the number of legs in the sensor. The packing density of the thermoelement legs, as can be seen from formula (2), also affects the response speed.

2. Calculation of the main parameters of thermoelectric microcalorimetric sensors

The parameters that need to be determined can be calculated as follows:

1) By definition, the volt-watt sensitivity is the ratio of the EMF of the microcalorimeter sensor E to the thermal power W released in the microcalorimeter reaction chamber.

$$\gamma = \frac{E}{W} \tag{3}$$

The thermoEMF of thermoelement legs *n*

$$E = \alpha \Delta T n \tag{4}$$

where α is the Seebeck coefficient.

Thermal power released in the microcalorimeter reaction chamber:

$$W = \chi \frac{S}{L} \Delta T n \tag{5}$$

where χ is thermal conductivity, S is cross-sectional area of the leg, L is leg length.

Therefore,

$$V = \frac{\alpha}{\chi} \cdot \frac{L}{S} \tag{6}$$

2) The thermopile resistance R is calculated by the formula:

$$R = \frac{1}{\sigma} \cdot \frac{L}{S} \cdot n \tag{7}$$

where σ is electric conductivity.

3) The response speed of thermopile τ:

$$\tau = \frac{c}{\chi} \cdot \frac{L}{S} \cdot \frac{1}{n} \tag{8}$$

where c is heat capacity.

4) This paper considers thermoelectric metal and semiconductor sensors with star-shaped and radial arrangement of thermoelements. The number of thermoelement legs n for the design is calculated individually.

Let us calculate the packing density of a metal (thermocouple) thermoelectric sensor with radial arrangement of legs (Figs. 2 and 3).

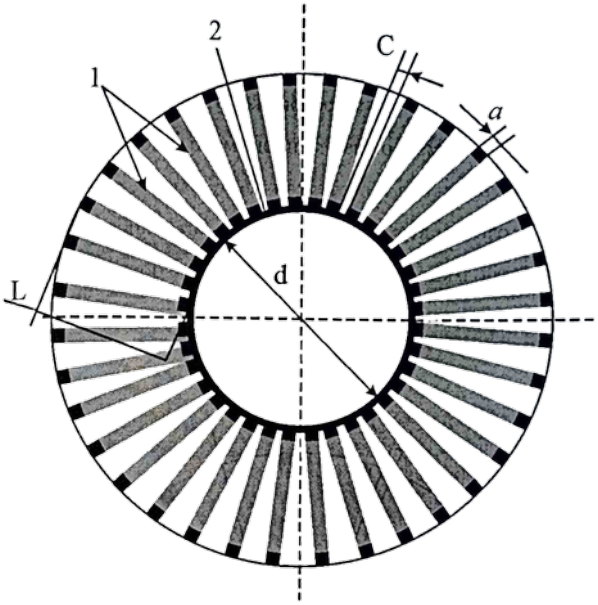


Fig. 2. Thermocouple sensor with radial arrangement of legs (top view):
1 –plates with thermocouples, 2 – reaction chamber, a – thickness of thermocouple leg,
C –distance between the legs from the chamber side, L – effective length of the leg.

Fig. 2 shows a top view of this sensor. Plates 1 with thermocouples are radially arranged around the reaction chamber 2. Let us count the number of plates.

$$n_1 = \frac{\pi d}{a+c} \tag{9}$$

Fig. 3 shows a measuring cell with a sensor mounted with radial arrangement of thermocouple legs. The thermocouple legs in plate 3 are connected by a snake.

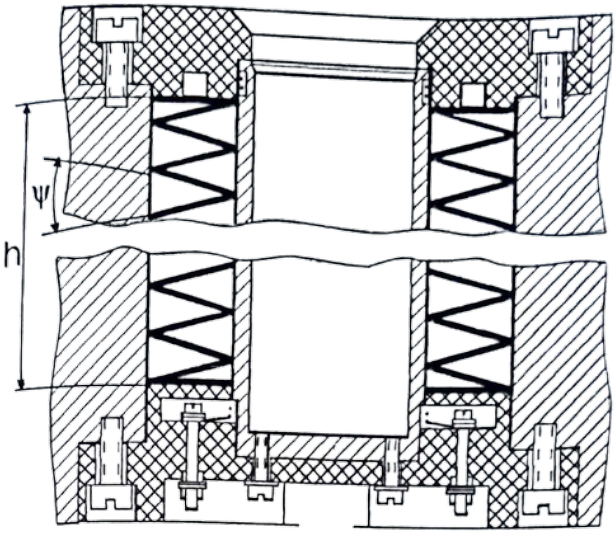


Fig. 3. Measuring cell with a sensor mounted with radial arrangement of thermocouple legs (side view):
h – sensor height; ψ – angle between thermocouple legs in case of their vertical arrangement.

The number of thermocouple legs n_2 in each such plate:

$$n_2 = \frac{h}{L \cdot \sin\frac{\varphi}{2}} \tag{10}$$

Thus, the number of thermocouple legs in such a sensor:

$$n = n_1 \cdot n_2 = \frac{\pi d}{a+c} \frac{h}{L \cdot \sin \frac{\varphi}{2}} \quad (11)$$

Since the number of thermocouple legs must be an integer, when finding the packing density n in the values n_1 and n_2 only the integer part should be left.

The design of a thermoelectric metal sensor with star-shaped arrangement of legs is presented in Figs. 4 and 5.

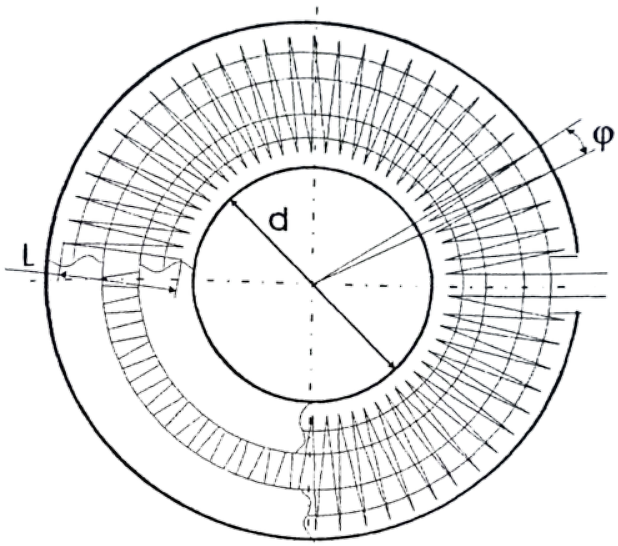


Fig. 4. Thermocouple sensor with star-shaped arrangement of legs (top view): d – chamber diameter; L – length of the thermocouple leg; φ – angle between the thermocouple legs in the case of their vertical arrangement.

Fig. 4 shows the design of a thermoelectric metal sensor with star-shaped arrangement of legs (top view).

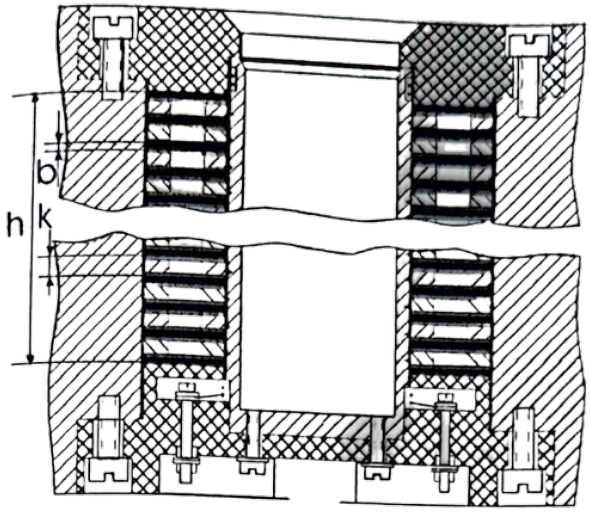


Fig. 5. Measuring cell with a sensor mounted with star-shaped arrangement of thermocouple legs (side view): h – sensor height; b – insulation thickness; k – thermocouple thickness.

Fig. 5 shows the arrangement of thermopiles along the height of the reaction chamber. The number of thermocouple legs of one thermopile in the design of a thermoelectric metal sensor with star-

shaped arrangement of legs is calculated using the formula

$$n_1 = \frac{\pi d}{L \cdot \sin \frac{\psi}{2}} \tag{12}$$

The number of thermopiles:

$$n_2 = \frac{h}{b+k} \tag{13}$$

Packing density of such a sensor is calculated by the formula:

$$n = \frac{\pi d}{L \cdot \sin \frac{\psi}{2}} \cdot \frac{h}{b+k} \tag{14}$$

Next, we will calculate the packing density for semiconductor microcalorimetric sensors with star-shaped and radial arrangement of semiconductor legs.

The design of semiconductor sensors with radial arrangement of semiconductor legs is shown in Figs. 6 and 7.

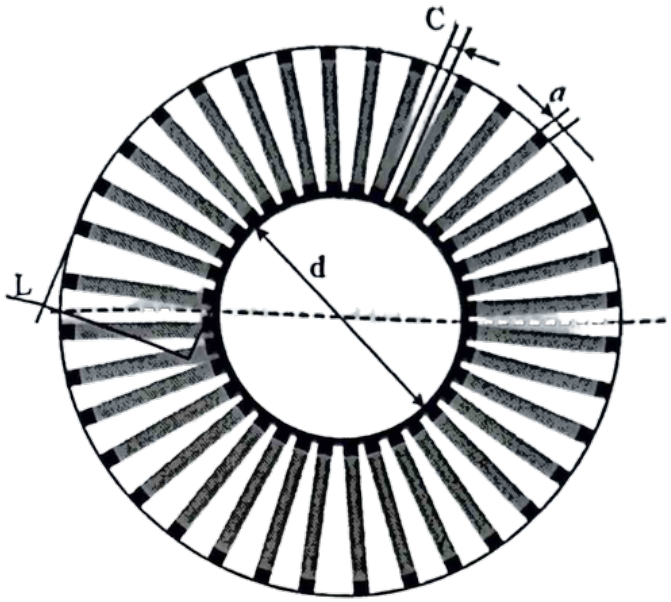


Fig. 6. Semiconductor sensor with radial arrangement of leg (top view):
a –thickness of thermocouple leg; C – distance between the legs;
L – length of the leg.

Number of thermopiles in such a sensor:

$$n_1 = \frac{\pi d}{a+c} \tag{15}$$

Number of blocks:

$$n_2 = \frac{h}{b+k} \tag{16}$$

Packing density:

$$n = \frac{\pi d}{a+c} \cdot \frac{h}{b+k} \tag{17}$$

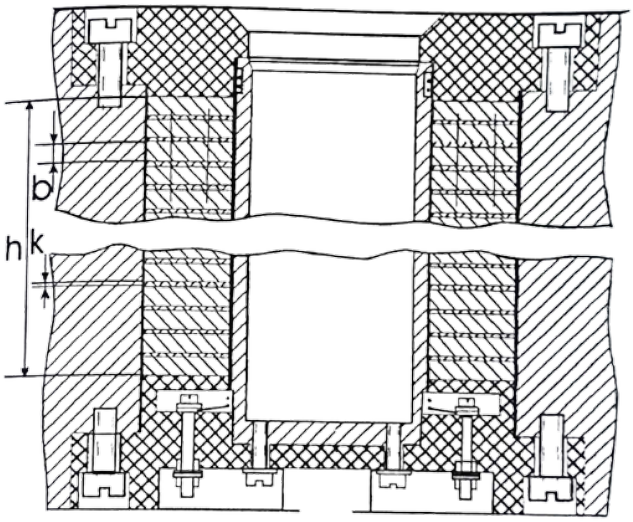


Fig. 7. Measuring cell with a sensor mounted with radial arrangement of semiconductor legs (side view): h – sensor height; b – insulation thickness; k – thermocouple thickness.

The design of semiconductor sensors with star-shaped arrangement of semiconductor legs is shown in Figs. 8 and 9.

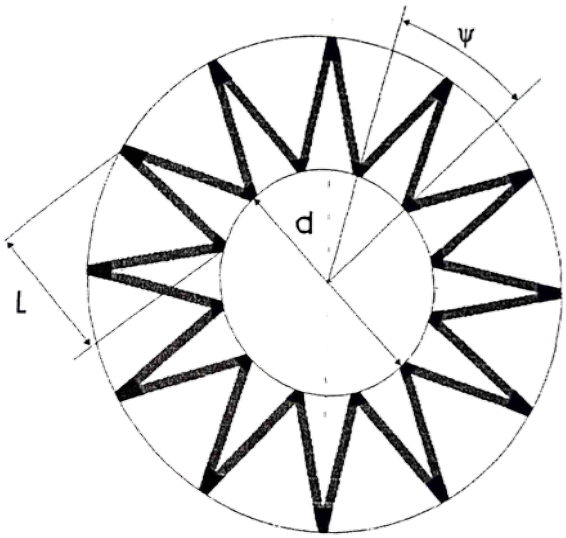


Fig. 8. Semiconductor sensor with star-shaped arrangement of legs (top view): d – chamber diameter; L – length of thermocouple leg; ψ – angle between legs.

Number of thermopiles in such a sensor:

$$n_1 = \frac{360}{\psi/2} \tag{18}$$

Number of blocks:

$$n_2 = \frac{h}{b+k} \tag{19}$$

Packing density:

$$n = \frac{360}{\psi/2} \cdot \frac{h}{b+k} \tag{20}$$

Thus, depending on the design of thermoelectric sensor, the packing density is calculated by the formulae (11), (14), (17), (20).

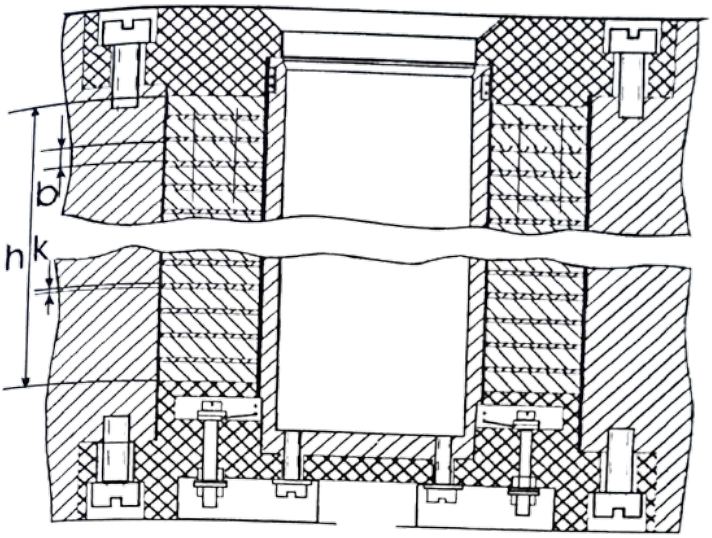


Fig. 9. Measuring cell with a sensor mounted with star-shaped arrangement of semiconductor legs (side view): h –sensor height; b –insulation thickness; κ – thermocouple thickness.

3. Algorithm for designing thermoelectric microcalorimetric sensors

Algorithm for designing thermoelectric sensors is shown as a block diagram in Fig.10.

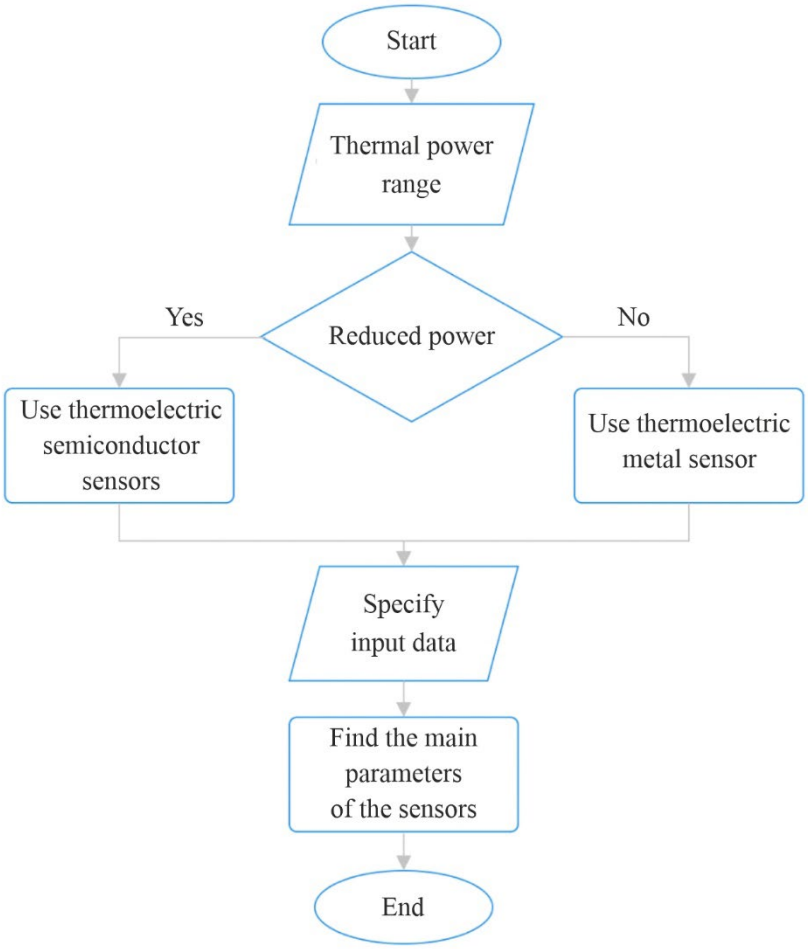


Fig. 10. Block diagram for designing thermoelectric microcalorimetric sensors.

4. Computer-aided design of thermoelectric sensors for microcalorimeters

In order to automate the design of thermoelectric sensors for microcalorimeters, a computer program was developed. The algorithm of the program is presented in Fig. 11 as a block diagram.

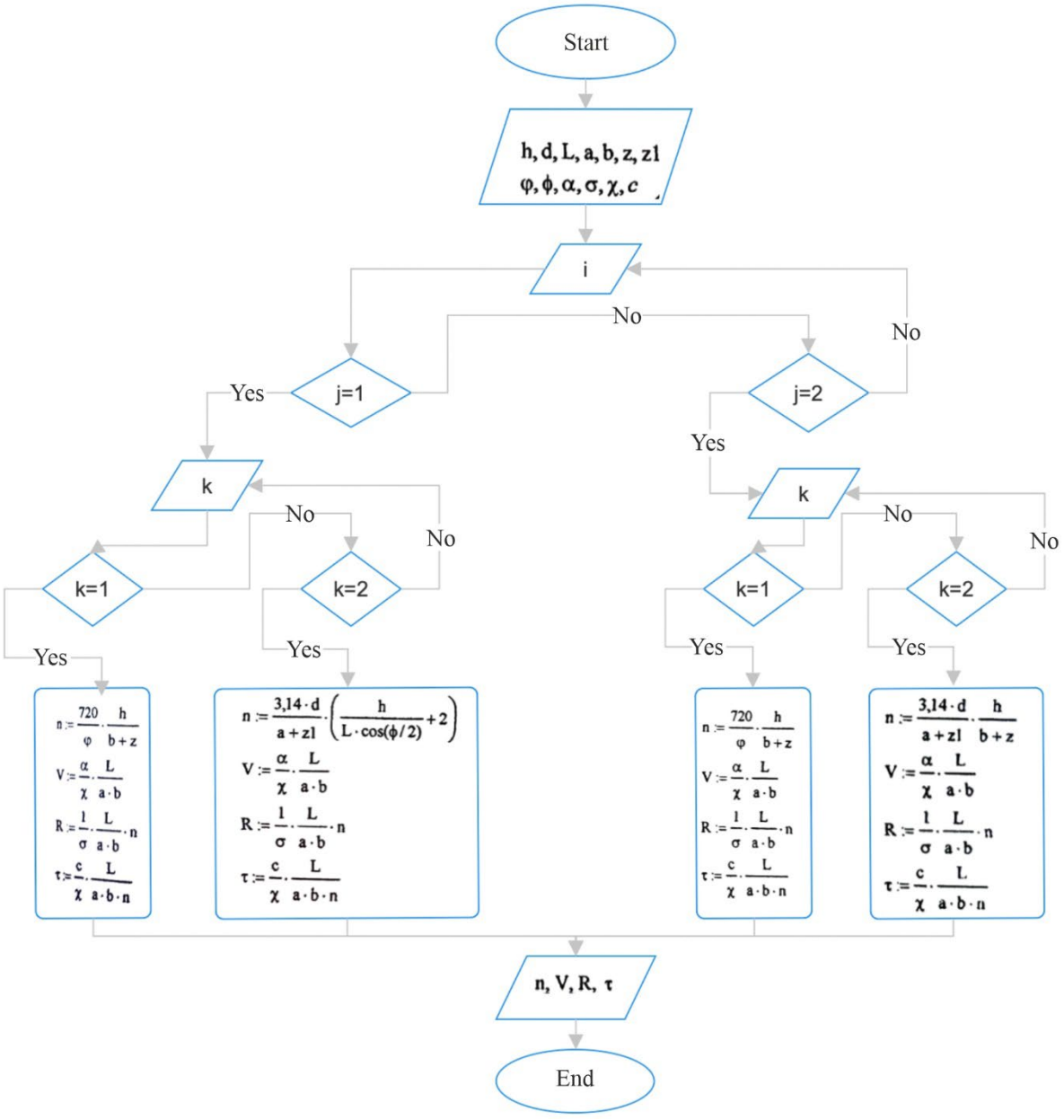


Fig. 11. Block diagram of calculating optimal values of the main parameters of thermoelectric sensors for microcalorimeters.

5. Examples of designing thermoelectric microcalorimetric sensors

We will design a sensor for reduced values of thermal power released in the reaction chamber, the sensitivity of which is 25 V/W. We will give an example of the calculation of a semiconductor microcalorimetric sensor with radial arrangement of thermoelements, made on the basis of extruded *Bi-Te* thermoelectric material.

Input data:

– height of the reaction chamber – 90 mm,
– diameter of the reaction chamber – 10 mm,
– cross-sectional area of the thermocouple leg – 0.9 × 0.9 mm^2,
– distance between thermopiles – 0.2 mm,
– distance between legs – 0.2 mm.

Physical properties of a pair of legs of Bi_2Te_3 semiconductors

$\alpha = 0.00018$ V/K;

$\sigma = 9000$ m^{-1}cm^{-1};

$$\chi = 0.018 \frac{\text{J}}{\text{K·cm·s}}$$

$$\text{c} = 0.15 \frac{\text{J}}{\text{K} \cdot \text{g}}$$

Calculated parameters:

– number of thermoelement legs – 1755,
– leg length – 10 mm,
– response speed – 28.93 s,
– resistance – 487 Ohm.

Next, we will calculate a thermoelectric metal sensor with a sensitivity of 0.25 V/W, whose legs are made of copper-constantan materials.

Input data:

– reaction chamber height – 90 mm,
– reaction chamber diameter – 10 mm,
– cross-sectional area of thermocouple leg – 0.9 × 0.9 mm^2,
– distance between thermopiles – 0.2 mm,
– angle between legs – 10°.

Physical properties of a pair of legs of Bi_2Te_3 semiconductors:

$\alpha = 0.00041$ V/K;

$\sigma =$ m^{-1}cm^{-1};

$$\chi = 0.23 \frac{\text{J}}{\text{K} \cdot \text{cm} \cdot \text{s}}$$

$$\text{c} = 0.31 \frac{\text{J}}{\text{K} \cdot \text{g}}$$

Calculated parameters:

– number of thermoelement legs – 2730,
– leg length – 10 mm,
– response speed – 1.2 s,
– resistance – 252 Ohm.

Based on the calculated parameters for a semiconductor microcalorimetric sensor with radial arrangement of thermoelements made on the basis of extruded *Bi-Te* material, as well as for a metal sensor with radial arrangement of thermocouple legs made on the basis of copper-constantan, it can be concluded that with the same length of the thermoelement legs, the sensitivity of the semiconductor

sensor is 100 times greater than that of the metal one, but the response speed of the metal sensor is 23 times greater than that of the semiconductor one.

Therefore, it can be concluded that when measuring low thermal powers in the reaction chamber of a microcalorimeter, it is better to use semiconductor sensors, since they have high sensitivity, and when measuring fast processes, it is better to use metal thermoelectric sensors.

Conclusions

1. A computer program has been developed to automate the design of thermoelectric microcalorimeter sensors, which provides the ability to enter key parameters and obtain the calculation of optimal values of the main characteristics of sensors, which simplifies and accelerates the design process of research equipment and microcalorimeters.
2. Software has been developed to automate the process of computer-aided design of highly sensitive thermoelectric microcalorimetric sensors, which makes it possible to improve the functionality of such sensors by implementing cutting-edge algorithms and computer simulation, and also provides significant progress in the accuracy of measurements and the response speed of such devices.
3. Thermoelectric microcalorimetric sensors for use in low-power reaction chambers have been designed and developed. The physical and mathematical aspects of the sensitivity and response speed of sensors made of *Bi-Te* semiconductor material and copper-constantan- based metal legs with appropriate geometric arrangement of the legs have been investigated.
4. It has been established that semiconductor sensors have significantly higher sensitivity compared to metal sensors with the same length of thermoelement legs, so their use is more effective when measuring low thermal powers. On the other hand, metal sensors demonstrate significantly better response speed, which makes them promising for use in fast processes.
5. The results obtained are the foundation for further development and improvement of thermoelectric sensors for microcalorimetric measurements, ensuring high sensitivity and accuracy in working with low-power energy processes.

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КОМП'ЮТЕРНЕ ПРОЕКТУВАННЯ ТЕРМОЕЛЕКТРИЧНИХ МІКРОКАЛОРИМЕТРИЧНИХ СЕНСОРІВ

У роботі виконано проектування і розробку термоелектричних мікрокалориметричних сенсорів для використання в малопотужних реакційних камерах. Досліджено фізичні та математичні аспекти чутливості та швидкодії сенсорів, виготовлених з напівпровідникового матеріалу Bi-Te і металевих віток на основі мідь-константану при відповідних геометричних розміщеннях віток. У роботі представлено алгоритм комп'ютерного проектування, зображений у вигляді блок-схеми, а також продемонстровано розробку програми для автоматизації процесу проектування, з подальшою імплементацією програмного забезпечення. Представлено практичні приклади розробки та аналізу розрахованих параметрів для двох типів сенсорів, щоб виявити їхні переваги у вимірюванні малих теплових потужностей та швидкоплинних процесів відповідно.

Ключові слова: мікрокалориметрія, термоелектричні мікрокалориметричні сенсори, комп'ютерне проектування сенсорів, програмне забезпечення.

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