Analysis of the applicability of the one-dimensional model for calculating thermal and thermoelectric processes in anisotropic bismuth thermoelements

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Abstract. The results of the temperature and electric potential numerical simulation in the model of an anisotropic thermoelement under thermal action typical for the experimental conditions on shock tubes are presented. The influence of the thermal conductivity anisotropy on the temperature distribution and the generated thermoelectric power is analysed. The results of solving the inverse problem - determining the heat flux from the calculated thermoelectric power are presented. The errors in calculating the heat flux on the basis of the one-dimensional model have been determined.

1. Introduction
Anisotropic thermoelements are widely used in thermoelectric power generators, cooling devices, heat flux sensors and radiation detectors [1]. The main parameter that determines the operating mode is the temperature distribution in the thermoelement. When thermoelements are used as generators of thermoelectric power or cooling devices, stationary thermal mode is the main one, and transient states are considered as undesirable [2]. In the case of using thermoelements as sensing elements of sensors, non-stationary thermal modes will be the main ones [3, 4].

A detailed analysis of thermal and thermoelectric phenomena is a very difficult task, which is due to the anisotropic nature of the kinetic coefficients and the nonlinearity of the system of equations [5, 6]. For this reason, a one-dimensional model is widely used to describe the main thermoelectric processes in anisotropic thermoelements [1]. This approach is often used at a fixed temperature of the working and rear surfaces of the thermoelement, when the effect of thermal conductivity anisotropy is small. In the case of using thermoelements as sensing elements of thermal sensors, a heat flux acts on the working surface (Neumann boundary condition), and the rear boundary is in thermal contact with the substrate (both Dirichlet and Neumann boundary condition). In this case, the assumption of a small effect of the thermal conductivity anisotropy requires additional verification.

In this paper, based on the numerical solution of the complete system of equations of thermal conductivity and electrical conductivity [1], an analysis of the applicability of the one-dimensional model under the conditions of unsteady thermal regimes of anisotropic thermoelements made of bismuth is presented. The characteristic time and heat flux through the working surface correspond to two typical conditions of experiments on shock tubes with different process times and heat transfer rates [7]. In the case of studying heat transfer upon reflection of a shock wave from the end-wall of the shock tube, the characteristic time of the process is \( t \sim 1 \mu s \). In the first phase, a reflected shock wave is formed, accompanied by a rapid increase of the heat flux. In the second phase, the cooling of the
heated near-wall gas layer begins, which is accompanied by a decrease of the heat flux $q_0 \sim 1/\sqrt{t}$ [8]. In the case of studying heat transfer with an external supersonic gas flow around the model, first there is an increase in the heat flux to the surface of the body, which corresponds to the phase of establishing the flow. In the second phase corresponding to the stationary flow regime, the heat flux remains constant during the time $t \sim 1\text{ms}$ [7].

The sensing element of the thermal sensor (figure 1a) is a battery of series-connected anisotropic thermoelements 1 cut from a bismuth single crystal, fixed on a mica substrate 2 and separated from each other by strips of lavsan 3. Wires 5 are soldered to the side thermocouples to connect to the oscilloscope. When the working surface of thermoelements is heated, a thermoelectric field appears in them, creating a thermoelectric power, which is output to an external circuit and recorded by an oscilloscope.

![Figure 1](image)

**Figure 1.** The design of the thermal sensor based on anisotropic thermoelements (a), model of the sensor based on anisotropic thermoelements (b).

2. **Mathematical models**

Further, two models of anisotropic thermoelement are considered. The first model uses a complete system of equations for thermal conductivity and electrical conductivity, taking into account the anisotropy of the coefficients of thermal conductivity, electrical conductivity and thermoelectric power. In the second simplified model, it is assumed that thermoelements are sufficiently long and edge effects can be neglected, and the temperature depends only on the transverse coordinate $y$. When calculating the thermoelectric power, only the transverse component of the thermoelectric field is taken into account $\sim \alpha_{xy} \frac{dr}{dy}$.

Since all thermoelements in the sensor are in the same thermal conditions, we will further consider a single thermoelement (figure 1b). Due to the symmetry of the crystal structure, the distribution of temperature and electric potential in all vertical sections is identical. Therefore, the computational domain is represented by connected rectangles corresponding to a bismuth thermoelement (1), a mica substrate (2), and a model element (3). Damage to the crystal structure of the thermoelement material during soldering of adjacent thermoelements and the resulting decrease in thermoelement are not taken into account. Typical $2 \times 0.2\text{mm}$ ($l/h = 10$) and $7 \times 0.4\text{mm}$ ($l/h = 17.5$) thermocouples are considered. The thickness of the substrate (2) and the model element (3) is selected equal 0.2 mm. The heat flux $q_0(t)$, which reproduces typical experimental conditions (black curve in Fig. 5), acts on the working surface of the thermoelement, the side faces of the thermoelement are thermally insulated, and all surfaces of the thermoelement are electrically insulated.

In the first model, the distribution of temperature $T(x,y)$ and electric potential $\varphi(x,y)$ is found from the solution of the system of equations [1]:

$$\text{equations}$$
$$C \rho \frac{dT}{dt} = \text{div} q$$

$$\text{div} j = 0$$

(1)

where $q$ is the heat flux and $j$ is the electric current, $T$ is temperature, $\lambda$, $\sigma$, $\alpha$ – the tensors of thermal conductivity, electrical conductivity and thermoelectric power. The generated thermoelectric power $\Delta \varphi$ is recorded between the extreme points on the rear side of the thermoelement. The calculation uses the following values of the tensor of thermal conductivity, electrical conductivity and thermopower:

$$\lambda = \begin{bmatrix} 8.17 & -1.28 \\ -1.28 & 7.72 \end{bmatrix} \text{W/m} \cdot \text{K}, \quad \sigma = \begin{bmatrix} 8.38 & -0.95 \\ -0.95 & 8.04 \end{bmatrix} \cdot 10^5 \text{1/Ohm} \cdot \text{m}$$

$$\alpha = \begin{bmatrix} -75.66 & -24.62 \\ -24.62 & -84.34 \end{bmatrix} \cdot 10^{-6} \text{V/K}$$

(2)

In the second model, the temperature distribution is found from the solution of the one-dimensional nonstationary heat transfer equation:

$$C \rho \frac{dT}{dt} = \frac{\partial}{\partial x} \left( \lambda \frac{\partial T}{\partial y} \right)$$

(3)

The generated thermoelectric power is determined by the expression:

$$\Delta \varphi_x = \alpha_{xy} \Delta T \frac{l}{h}$$

(4)

where $\alpha_{xy}$ – the off-diagonal element of the thermoelement tensor, $l/h$ – the ratio of the length to the thickness of the thermoelement [1]. The equations are solved numerically in the COMSOL Multiphysics package.

3. Results

Figure 2 shows the temperature field in the thermoelement and substrate 2 mm long (a) and 7 mm long (b) at time moment $t = 5 \text{ ms}$. It can be seen that due to the anisotropy of the thermal conductivity of bismuth, the isotherms are S-shaped, and an increase in the thermoelement length reduces the relative influence of edge effects. With further heating, the regions of deviation of isotherms from straight lines expand and in a stationary thermal regime they take the form of inclined straight lines. The rotation angle of the isotherms relative to the working surface is proportional to the ratio of the off-diagonal to the diagonal terms of the thermal conductivity tensor.

![Figure 2](image)

Figure 2. Temperature field in the thermoelement and substrate 2 mm long (a) and 7 mm long (b) at time moment $t = 5 \text{ ms}$.

Figure 3 shows the temperature distribution along the working and rear surfaces of the thermoelement with a length 2 mm and 7 mm. Figures (a) and (b) correspond to the case of shock wave reflection, Figures (c) and (d) correspond to the external flow around the body. In the first case, the curvature of isotherms is observed only near the ends of thermoelements; in the rest of the region, the temperature distribution is one-dimensional. In the case of a longer heating, the region of edge effects is much larger.
Figure 3. Temperature distribution along the working surface $T_h$ and rear surface of the thermoelement $T_0$ 2 mm long (a), (c) and 7 mm long (b), (d) at the time moment $t = 5 \mu s$ (a) and (b), $t = 5 ms$ (c) and (d).

The generated thermoelectric power is an integral quantity that makes it possible to estimate the effect of the anisotropy of properties on the whole. Figure 4 shows the thermoelectric power calculated using both models for two variants of the heat flux. At a short heating time, despite a slight bending of the isotherms (figure 3a and 3c), the difference in the calculated thermopower is significant (figure 4a); for the second heating variant, the difference is smaller (figure 4b).

Figure 4. Thermoelectric power for different variants of the heat flux, calculated using two variants of the thermoelement model.
When using anisotropic thermoelements as sensitive elements of sensors, the main task is to estimate the error when solving the inverse problem - calculating the heat flux from the electrical signal of the sensor. For this, you can use the method proposed in [4, 9]. Figure 6 shows the heat flux set and calculated using the [4] method. It can be seen that, in case (a), the difference between the calculated heat flux based on the electric signal and the specified $q_h$ for a thermoelement 2 mm long is $\approx 10\%$, and 7 mm long is no more than 5%. In this case, with an increase in the length of the thermoelement, the curves asymptotically converge to the specified $q_h$. In the case of prolonged heating, the difference between both curves from $q_h$ is $\approx 5\%$, however, the shape of the heat flux curve calculated from the signal of a short thermoelement slightly differs from $q_h$. For a thermoelement 7 mm long, the calculated heat flux reproduces $q_h$ with sufficient accuracy.

![Figure 5](image)

(a) Specified heat flux $q_h$ and calculated using a one-dimensional model based on the electrical signal of thermoelements of various lengths.

(b)

4. Conclusion
The results of calculating the temperature fields in anisotropic thermoelements 2 mm and 7 mm long when heated by a heat flux corresponding to the reflection of a shock wave with a duration of $t \sim 1 \mu s$ and the establishment of an external supersonic flow around the body $t \sim 1 ms$. Heat flow curves were reconstructed from the calculated electrical signals of thermoelements. The error in calculating the heat flux based on the one-dimensional model for a thermoelement with a length of 2 mm is $\approx 10\%$, and for a thermoelement with a length of 7 mm does not exceed 5%.

References
[1] Rowe D M 2006 Thermoelectrics Handbook: Macro to Nano (CRC Press) pp 954
[2] Babin V P and Iordanishvili E K 1983 Non-stationary processes in thermoelectric and thermomagnetic energy conversion systems (M.: Nauka) pp 216 (in russian)
[3] Sapozhnikov S Z, Mityakov V Yu and Mityakov A V 2020 Heatmetry: The Science and Practice of Heat Flux Measurement (Springer International Publishing) pp 209
[4] Popov P A, Bobashev S V, Reznikov B I and Sakharov V A 2018 Tech. Phys. Lett. 44 (4) 316–9
[5] Bobashev S V, Popov P A, Reznikov B I, Sakharov V A 2016 Tech. Phys. Lett. 42 (5) 460–3
[6] Popov P A, Bobashev S V, Reznikov B I and Sakharov V A 2017 Tech. Phys. Lett. 43 (4) 334–7
[7] Popov P A, Sakharov V A, Lapushkina T A, Poniaev S A and Monakhov N A 2021 Phys.–Chem. Kin. in Gas Dyn. 22 (3) 1–11
[8] Fay J A, Kemp N H 1965 J. Fluid Mech. 21 (4) 659–72
[9] Dobrov Yu V, Lashkov V A, Mashek I Ch, Mityakov A V, Mityakov V Yu, Sapozhnikov S Z and Khoronzhuk R S 2021 Tech. Phys. 66 (2) 229–34