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The influence of the number of channels on the efficiency of permeable thermoelements from Bi-Te-Se-Sb materials

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The results of studies of permeable thermoelements are presented. The method of mathematical theory of optimal control and computer-aided design for solving multivariate optimization problems is described. Computer-aided calculation of parameters for permeable thermocouples based on Bi-Te-Se-Sb is done. The obtained results indicate the possibility of increasing the energy conversion efficiency by 1.2 - 1.5 times due to thermoelectric materials.

Key words: the material of thermoelement, thermoelectric conversion, COMSOL Multiphysics, functionally gradient material, Bi-Te-Se-Sb, engineering design.

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Introduction

Thermoelectric generators have been known in the engineering for less than two centuries, but their industrial application began relatively recently, almost simultaneously with the discovery of the first semiconductors. Thermoelectric conversion of thermal energy into electrical energy still requires greater popularization, especially in case of the growing need for alternative sources of electric energy [1, 2].

The cryogenic thermogenerators in medical devices used for implantation into the human body (IMD), such as cardiac pacemakers, defibrillators, drug dosing pumps and neurostimulators, are prospective. Most of these devices use the non-rechargeable batteries as the power-supply source. Therefore, the main limitation of such devices is the battery operational life.

Currently, the wide application of SCM with a maximum operating temperature of up to 280°C. This temperature is very high for bismuth telluride alloys, the basis of the semiconductor branches of the vast majority of SCM emitted. Long-term operation of SCM based on the specified material at temperatures above 300°C is impossible. This is what defines the SCM category based on this semiconductor as “low temperature SCM” [3].

One of the ways to expand the use of low-temperature thermoelectricity is to introduce new thermoelectric materials that are more efficient than traditional materials based on Bi_2Te_3, PbTe, Si-Ge. The first theoretical studies of permeable thermoelements for gas flows [4-6] indicated the perspective of their creation, since they predict an increase in the cooling factor of 30 - 40% [7] when cooling the air and an increase in the efficiency of generators by 20 - 30% [8] when used low-potential thermal energy of gases.

Therefore, in the study [9], for the more correct solution of such problems, the mathematical theory of optimal control was used for the first time and the research of permeable thermoelements in 1-D model of semiconductors was carried out, taking into account their temperature dependences, for homogeneous and functionally gradient materials (FGM). This made it possible to create a theory of permeable thermoelements with FGM and to point out the possibility of increasing the energy characteristics in the modes of generation of electric energy and cooling of heat carriers by 1.2 - 1.5 times.

A prospective direction for increasing the efficiency of thermoelectric energy conversion is the use of physical models of thermoelements, in which heat exchange with the source and heat sink is carried out not only through the joints of branches, which is characteristic of traditional thermoelements, but also in the volume of material of the branches.

Physical models use the effect of scale in the case of proportional use of the whole complex of studied properties. A physical model is an analog model in which there is a clear correspondence between the parameters of an object and a model of the same physical nature. In this case, the elements of the system are matched by physical equivalents that reproduce the structure, basic properties and ratios of the object under study. In the physical modeling, which is based on the theory of similarity, features of the experiment in nature are preserved, with the optimal range of change of the corresponding physical parameters.

The embodiments of such models are segmental thermoelements having channels for the heat carrier to flow through them. The presence of heat exchange in the volume of the branch increases the intensity of heat transfer, leads to the redistribution of temperature fields, potentials and heat fluxes, thus affecting the energy characteristics of the thermoelement. By controlling the thermophysical parameters (the rate of pumping of the heat carrier, the intensity of heat transfer, the density of electric current), it is possible to realize such operating conditions under which the energy efficiency of energy conversion will be improved.

The first theoretical studies of segmental thermoelements showed the prospect of their creation, forecasting an increase of the coefficient by 30-40% when cooling air and increasing the efficiency of generators by 20-30% when using low-potential thermal energy. However, such studies were performed for the simplest model of a thermoelement in one-dimensional approximation without taking into account the temperature dependences of the material parameters and the comutative heat transitions.

I. Physical model, mathematical description and results of solving the problem

For an inhomogeneous isotropic permeable thermoelectric environment in which there is a steady flow of heat, charged particles and energy caused by the presence of temperature gradients ∇Ti electrochemical potential $\nabla\zeta$ energy exchange and conversion processes are described by fundamental laws of energy and electric charge conservation.

In the stationary case, the temperature distribution T in the thermoelectric material is determined by the system of differential equation system in partial derivations

$$\nabla k\nabla T + \frac{i^2}{s} - t\vec{i}\nabla T - T\vec{i}\nabla_T a = 0\,, \qquad (1)$$

where $\vec{q} = -k\nabla T + aT\vec{i}$ – vector of heat flux density; $\vec{i} = -s\nabla z - sa\nabla T$ – vector of electric current density; a – coefficient of thermoEMF, s – electrical conductivity coefficient; k – coefficient of thermal conductivity.

The presence of heat exchange of a thermoelectric material with a heat carrier necessitates solving the problems (1) which are related to the indivisibility, motion and thermal conductivity equations for the heat carrier, which can be written in the following way:

$$\left.\begin{aligned}
&\mathrm{div}(r_t\vec{V}) = 0,\\
&r_t\vec{F} - \nabla p + m\nabla^2\vec{V} + \frac{1}{3}m\nabla(\mathrm{div}(\vec{V})) = 0,\\
&r_t\vec{F}\vec{V} + \mathrm{div}(\Lambda\vec{V}) + \mathrm{div}(k_t\nabla t) + r_t q_{\mathrm{V}} = 0,
\end{aligned}\right\} \qquad (2)$$

where r_t – the density of the heat carrier; $\vec{V}$ – heat carrier rate; $\vec{F}$ -mass force; p-pressure; Λ – voltage tensor; k_t – coefficient of thermal conductivity of the heat carrier; q_{V} – internal heat sources; U – internal energy.

It is advisable to carry out this task in specially designed computer programs such as Femlab, ANSYS, COMSOL Multiphysics.

3-D simulation of the generator thermoelement with the side heat exchange was carried out in the study [10] based on the COMSOL Multiphysics program. The temperature distributions in the material of the branch based on Bi-Te and the heat carrier (Fig. 1a), the velocity distribution of the heat carrier (Fig. 1b) and the distribution of the potentials, which allows to determine the thermodynamic characteristics of the transformation were obtained.

The results of the calculations indicate that with the use of side heat transfer large values of efficiency are achieved if the heat transfer at the level of 0.5 height of the branch, and other parts have thermal insulation. The data were obtained for other thermoelement constructions and the heat carrier temperatures, which vary in the range of 700 - 1100 K. The data indicate that the use of side heat transfer can give an efficiency improvement of 20 - 30% and an electric power of 40 - 50%.

The calculation data indicate the need to solve the multi-parameter optimization problem of finding the optimal conditions of operation of the thermoelement and maximum values of its energy characteristics. However, such multi-parameter optimization for the 3-D model is extremely difficult. The use of the 1-D model allows to perform multi-parameter optimization of energy characteristics of thermoelements, to identify such conditions of their operation, under which it is possible to achieve maximum values of energy conversion efficiency.

In the 1-D case, determining the energy characteristics of a permeable thermoelement is based on the solution of a system of differential equations for the heat carrier and the material of branches, branches n- i p-type of conduction, like:

$$\left.\begin{aligned}
&\frac{dT}{dx}=-\frac{\alpha\ j}{\kappa}T-\frac{q}{\kappa},\\
&\frac{dq}{dx}=\frac{\alpha^2 j}{\kappa}T+\frac{\alpha\ j}{\kappa}q+i^2\rho-\frac{\alpha_T P_K N_K l^2}{\left(S-S_K\right)j}\left(T-t\ \right),\\
&\frac{dt}{dx}=\frac{\alpha_T P_K N_K l}{Vc_P S_K}\left(T-t\ \right).
\end{aligned}\right\}\qquad(3)$$

where T, t – the temperature of the branch material and the heat carrier at the x - point; $j=il$ – the current density of the electric flux; l – the height of branches of thermoelement; i – the density of the electric flux; $q=\frac{1}{j}\left(\alpha jT-\kappa\frac{dT}{dx}\right)$ – the specific heat flow; $x=\frac{\mathrm{x}}{l}$ – dimensionless coordinate; S_K – the cross-sectional area of all channels; S – the cross section of the branch together with the channels; P_K – the perimeter of the channel; N_K – the number of channels in the branch; V – the mass velocity of the hear carrier in the channels; α_T – the coefficient of heat transfer in the channel.

To solve the optimization issue of finding the optimal conditions of operation of the thermoelement, the Pontryagin maximum principle of mathematical theory of optimal control, which gives the necessary conditions for optimality, was used in the studies:

1) optimal values of the specific current density in the branches of the thermoelement j should satisfy the equation:

$$-\left[\frac{\partial J}{\partial j}\right]_{n,p}+\sum_{n,p}\int_0^1\left[\psi_1\frac{\partial f_1}{\partial j}+\psi_2\frac{\partial f_2}{\partial j}+\psi_3\frac{\partial f_3}{\partial j}\right]_{n,p}dx=0,\ (4)$$

where J – the functional that characterizes the efficiency of the energy conversion process (efficiency for generators, cooling coefficient for cooling, etc.); $\left(f_1,f_2,f_3\right)_{n,p}$ – the right hand side of the equation (1), $\psi=\left(\psi_1,\psi_2,\psi_3\right)_{n,p}$ – vector impulse function [12], which is determined by the solution of the auxiliary system of differential equations:

$$\left.\begin{aligned}
&\frac{d\psi_1}{dx}=\frac{\alpha\ j}{\kappa}R_1\psi_1-\left(\frac{\alpha\ j}{\kappa}R_2-\frac{\alpha_e l}{\left(S-S_K\right)j}\right)\psi_2+\frac{\alpha_T P_K^1 N_K}{Gc_P}\psi_3,\\
&\frac{d\psi_2}{dx}=\frac{j}{\kappa}\psi_1-\frac{\alpha\ j}{\kappa}\psi_2,\\
&\frac{d\psi_3}{dx}=-\frac{\alpha_T P_K^1 N_K l}{\left(S-S_K\right)j}\psi_2-\frac{\alpha_T P_K^1 N_K}{Gc_P}\psi_3,
\end{aligned}\right\}_{n,p}\qquad(5)$$

where:

$$\left.\begin{aligned}
&R_1=1+\frac{d\ln\alpha}{dT}T-\frac{d\ln\kappa}{dT}\left(T+\frac{q}{\alpha}\right),\\
&R_2=R_1+\frac{\kappa}{\alpha^2\sigma}\frac{d\ln\sigma}{dT}+\frac{d\ln\kappa}{dT}\left(T+\frac{q}{\alpha}\right).
\end{aligned}\right\}_{n,p}$$

2) the optimal values of the parameters that are determined, $w_i=(w_1,...,w_r)$, are calculated from the system of integral-differential equations:

$$-\left[\frac{\partial J}{\partial w_i}\right]_{n,p}+\sum_{n,p}\int_0^1\left[\psi_1\frac{\partial f_1}{\partial w_i}+\psi_2\frac{\partial f_2}{\partial w_i}+\psi_3\frac{\partial f_3}{\partial w_i}\right]_{n,p}dx=0,\ i=1,...,r.\qquad(6)$$

Analyzing the results obtained using the method of sequential approximations and the methods of solving the systems of differential equations (3) and (5), Newton's method for solving systems of integral-differential equations (6) a computer program for designing a permeable thermoelement was developed [10].

Temperature dependences of parameters a, s, k materials based on Bi-Ti-Se-Sb (fig. 2) were used for calculations.

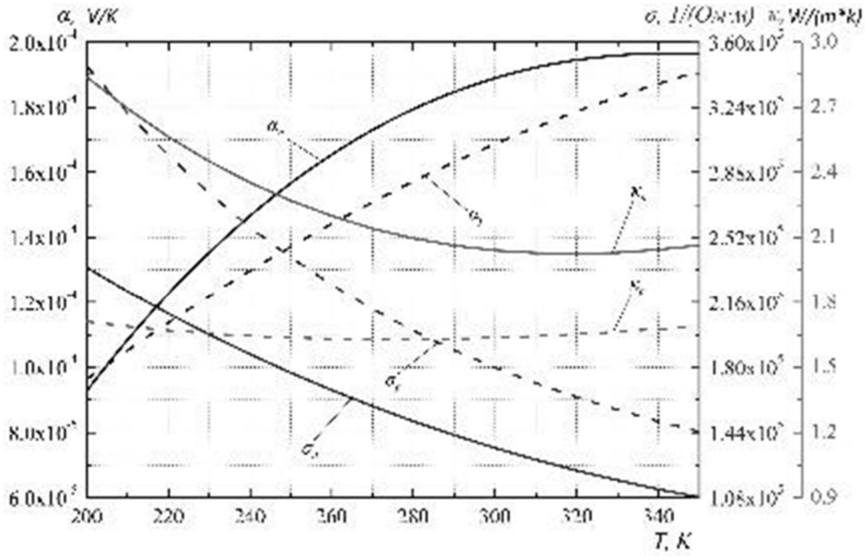

Fig. 2. Temperature dependences of parameters of the materials based on Bi-Te-Se-Sb .

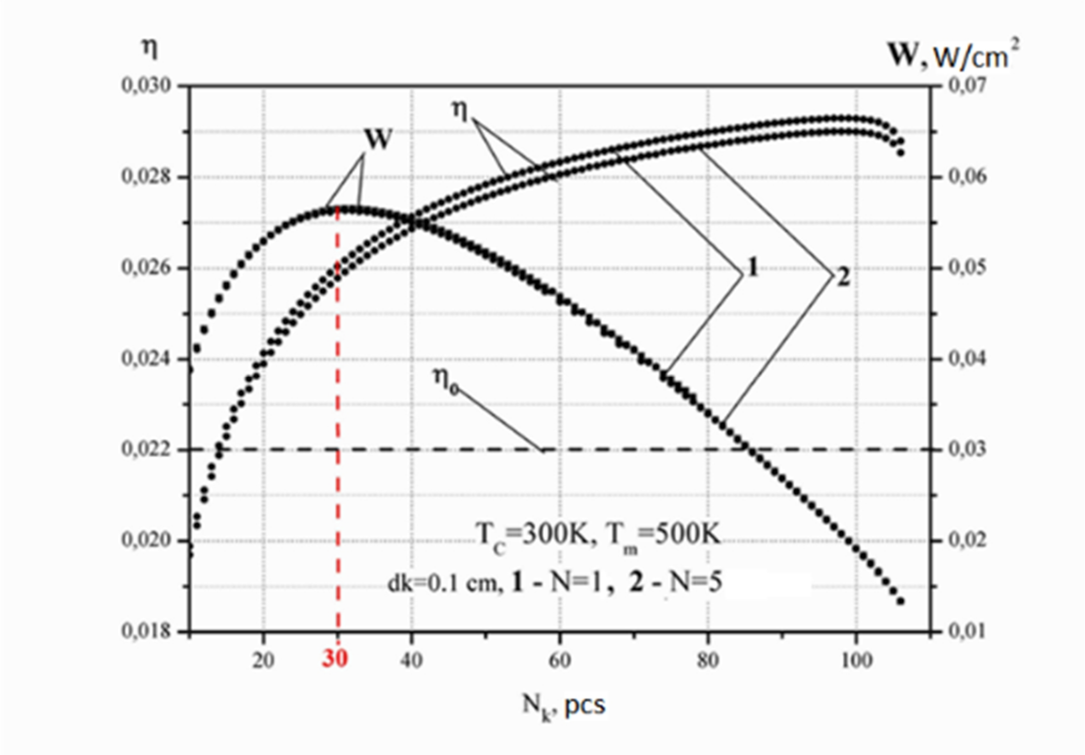

Fig. 3. The dependencies of efficiency and power generated W on the number of channels $N_{k.}$

Results of calculations of permeable generator thermoelement from materials based on Bi-Te-Se-Sb from the number of channels 1 i 2 segment penetrating thermoelement in the optimal conditions are shown in fig.3. It is seen that the efficiency increases with the increase in the number of channels and goes to saturation. But even at its limit values corresponding to the boundary porosity (85%) of the material, the efficiency of the thermoelement begins to decrease. Specific electrical power has a maximum, in this case at 30 channels per 1 cm^2. Therefore, the rational number of channels per unit area will be in the range of 30 - 60 units. Comparison with the efficiency of the classical thermoelement η_0, operating under similar conditions, also indicates the possibility of increasing the energy conversion efficiency by about 30-50%.

Conclusions

The possibility of using low-temperature generators is analyzed and it is said that physical models are used to understand the essence of physical processes in the studied materials, which include theoretical calculation with subsequent design of the material, where the circulating heat carrier flows through the branches of the semiconductor material.

For the investigated materials of type - Vi-Te-Se-Sb, the degree of influence of structural parameters (diameter of channels and their number, height of branches and number of segments) is calculated. The most optimal conditions for their operation in terms of thermoelement efficiency are determined. The best values of influencing parameters are named, by means of which it is possible to determine the characteristic material values for a given type of thermoelement.

The comparison on the thermodynamic efficiency of energy conversion with traditional thermoelements showed the possibility of increasing the efficiency by 1.2 - 1.5 times.

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Вплив числа каналів на ефективність проникних термоелементів з матеріалів на основі Bi-Te-Se-Sb

Представлені результати досліджень проникних термоелементів. Описано метод математичної теорії оптимального управління та комп'ютерного проектування для вирішення багатофакторних оптимізаційних задач. Зроблено комп'ютерний розрахунок параметрів для проникних термоелементів, що виготовлені на основі Bi-Te-Se-Sb. Отримані результати свідчать про можливість збільшення ефективності перетворення енергії в 1,2 - 1,5 рази за рахунок термоелектричних матеріалів.

Ключові слова: Матеріал термоелементу, термоелектричне перетворення, COMSOL Multiphysics, функціонально-градієнтний матеріал, Bi-Te-Se-Sb, проектування.