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COMPUTER DESIGN OF PERMEABLE FUNCTIONALLY GRADED MATERIALS FOR THERMOELEMENTS IN ELECTRIC ENERGY GENERATION MODE

Based on the Pontryagin maximum principle of optimal control theory, a methodology for designing optimal functionally graded materials (FGM) for permeable thermoelectric elements is presented. An algorithm and a computer program have been created, which have been tested for finding the optimal FGM for n- and p-type legs based on Bi-Te-Se-Sb. It has been shown that under optimal conditions, 1.3 – 1.7 fold efficiency increase is achieved when using permeable generator thermoelements with FGM compared to traditional thermoelements with homogeneous legs.
Key words: computer design, permeable structures.

Introduction

The possibilities of wide practical application of thermoelectricity for creation of electric energy sources depend primarily on their efficiency. The main ways of increasing the efficiency are considered to be, first of all, improvement of the figure of merit of thermoelectric materials $Z = \alpha^2\sigma/\kappa$ (α – thermoEMF, σ – electrical conductivity, κ – thermal conductivity) and reduction of losses in heat supply and removal systems.

Analysis of the literature. The main methods for increasing the figure of merit of thermoelectric materials were formulated by A.F. Ioffe in the middle of the last century [1]. They come down to optimizing the thermoelectric material by appropriate doping with active impurities to achieve maximum values of $\alpha^2\sigma$ and doping the material with isovalent substitution impurities to reduce thermal conductivity. Such methods were applied to a number of materials, which led to an increase in the figure of merit and, accordingly, contributed to the widespread use of thermoelectricity.

However, in the last decade, despite numerous studies, further growth of the figure of merit of thermoelectric materials has been insignificant. It becomes obvious that the above methods have exhausted themselves. There is a need to find new ways to increase efficiency. Therefore, more and more attention is paid to the study of one-dimensional and filament structures, film materials and quantum well composites. Unfortunately, to date, these methods have not yet yielded significant practical results in thermoelectricity. Thermoelectric materials with programmable functional inhomogeneity (FGM) are also being studied, which increase the efficiency due to the use of volumetric thermoelectric effects and the correct consideration of the temperature dependence of material properties [2, 3]. Today, this method is considered the most realistic for increasing the efficiency of thermoelectric energy conversion.

The improvement of the heat exchange system consists in the intensification of heat exchange, which can be implemented in the case when heat is supplied or removed not only through the surfaces of the hot and cold junctions, but also by using the volume of thermoelement legs. Such thermoelements are made permeable to heat carriers, due to which they are usually called permeable [6 – 8].

I.V. Zorin in his author's certificates was one of the first to point out the possibility of increasing the efficiency of thermoelectric energy conversion by using permeable thermoelements. A consistent research of the capabilities of thermoelements with permeable legs was pursued in Ukraine. The paper [9] presents a classification of variants of physical models of such thermoelements. Studies of extreme energy characteristics of a generator thermoelement made of permeable legs when passing a heat carrier from the hot to cold junctions confirmed the possibility of a significant efficiency increase [10], where such problems were solved for a homogeneous material of the thermoelement legs without taking into consideration the temperature dependences of its parameters.

Since efficiency increase is achieved both by using thermoelement legs that are permeable to heat carrier and by using inhomogeneous materials, research into the possibilities of the combined influence of these two factors on the efficiency of energy conversion is promising. A new optimization problem arises, which consists in the fact that it is necessary to find such optimal parameters (heat carrier flow rate, electric current density, etc.) that are consistent with the optimal distribution function of the inhomogeneity of the thermoelectric materials of legs (FGM), at which the highest value of the efficiency of the generator thermoelement is achieved.

Model of a permeable FGM thermoelement, mathematical description and method of solving the problem

The physical model of a permeable FGM thermoelement, operating in the electric energy generation mode, is shown in Fig. 1. It contains *n*- and *p*-type legs, the properties of which change with the *x* coordinate due to their dependence on the temperature $T(x)$ and the concentration of current carriers $\xi(x)$. The temperature of the heat carrier supplied to the thermoelement is T_m, the temperature of the cold junctions of the thermoelement is T_c. The presence of contact resistances r_0 at the junctions of connecting plates with the thermoelement legs is taken into consideration. The side surfaces of the legs are insulated. The heat carrier is pumped through the thermoelement. Heat from the heat carrier is transferred to the material through heat exchange with the inner surface of the channels of the legs and creates a temperature distribution in the material of the legs. The action of thermoelectric effects leads to the occurrence of thermoEMF.

The stationary distribution of temperatures $T(x)$ and heat flows $q(x)$, heat carriers $t(x)$ in the legs will be found by solving the system of differential equations

$$\left.\begin{aligned} &\frac{dT}{dx} = -\frac{\alpha\ j}{\kappa}\ T - \frac{j}{\kappa} q, \\ &\frac{dq}{dx} = \frac{\alpha^2 j}{\kappa} T + \frac{\alpha\ j}{\kappa} q + j\rho + \frac{\alpha_e l}{\left(S - S_K\right) j}\left(t - T\right), \\ &\frac{dt}{dx} = \frac{\alpha_e}{Gc_p}\left(t - T\right), \end{aligned}\right\}_{n,p} \tag{1}$$

where $\alpha_{n,p} = \alpha_{n,p}(T(x),\xi_{n,p}(x))$, $\kappa_{n,p} = \kappa_{n,p}(T(x), \xi_{n,p}(x))$, $\rho_{n,p} = \rho_{n,p}(T(x), \xi_{n,p}(x))$ are the Seebeck coefficient, thermal conductivity and electrical resistivity of the material of *n*- and *p*-type legs that depend on the concentration of current carriers $\xi_{n,p}(x)$ and temperature $T(x)$; $x = \frac{x}{l}$ is dimensionless coordinate; $\alpha_e = \alpha_T \Pi_K^1 N_K l$ is effective coefficient of heat transfer, α_T is coefficient of heat transfer of heat carrier in the channels, Π_K^1 is the perimeter of one channel, N_K is the number of channels in the leg, l is the height of thermoelement legs; t is the temperature of heat carrier at point x; T is the temperature of leg at point x; $j = il$; i is current density ($i = \frac{I}{(S - S_K)}$); S – is the cross-sectional area of leg together with the channels; S_K is the cross-sectional area of all channels of the leg; G is mass flow rate of heat carrier; c_p is heat capacity of heat carrier.

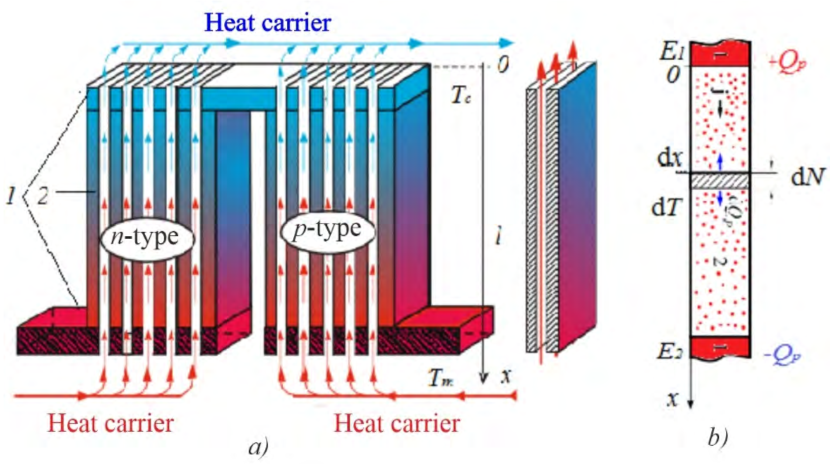

Fig. 1. Model of a permeable generator thermoelement (a): 1 – connecting plates; 2 – legs of n and p conductivity types; (b) – volumetric effects in the legs of an inhomogeneous thermoelement: 1 – electrical contact, 2 – thermoelectric material.

The main task is to find mutually consistent optimal distributions of the current carrier concentrations in the material of the legs $\xi_{n,p}(x)$, the coolant flow rate G and the electric current density j, at which the maximum efficiency is achieved for the given temperatures of the cold junctions T_c, the heat carrier T_m and under the condition of thermal insulation of the hot junctions. Therefore, the boundary conditions for the system of differential equations (1) are as follows:

$$t_{n,p}(1) = T_m, \quad q_n(1) + q_p(1) = 0, \quad T_n(1) = T_p \tag{1}$$

$$T_{n,p}(0) = T_c, \tag{2}$$

The task of achieving maximum efficiency:

$$\eta = \frac{W}{Q_p} \tag{3}$$

where $W=\sum_{n,p}\left\{Gc_P\left(T_m-t(0)\right)+\left(q(0)+j\frac{r_0}{l}\right)\frac{j\left(S-S_K\right)}{l}\right\}$ is electric power generated by thermoelement; $Q_p=\sum_{n,p}Gc_p\left(T_m-T_c\right)$ is thermal energy of the heat carrier; r_0 is contact resistance, can be conveniently reduced to the task of achieving the minimum of functional:

$$J=\ln\left[\sum_{n,p}\left\{G_{C_p}\left(T_m-T_C\right)\right\}\right]-\ln\left[\sum_{n,p}\left\{G_{C_p}\left(T_m-t(0)\right)+\left(q(0)+j\frac{r_0}{l}\right)\frac{jS}{l}\right\}\right] \tag{4}$$

In the language of optimal control theory, the optimization problem is to determine the heat carrier flow rate *G*, the generating current density *j*, and the carrier concentration functions in the leg material $\xi_{n,p}$(x) (or the concentration value $\xi_{n,p}$, for the case of searching for an optimally homogeneous leg material), which, under the constraints imposed by the system (1), (2), impart to the functional *J* the smallest value.

To solve such an optimization problem, the Pontryagin maximum principle [10] of mathematical optimal control theory is used. For the minimum of *J* the following conditions must be met:

1. Current density must satisfy the equation:

$$-\frac{\partial J}{\partial j}+\sum_{n,p}\int_0^1\frac{\partial H\ (\psi,T,q,t,j,G)}{\partial j}dx=0 \tag{5}$$

2. Heat carrier flow rate in the channels must satisfy the equation:

$$-\frac{\partial J}{\partial G}+\sum_{n,p}\int_0^1\frac{\partial H\ (\psi,T,q,t,j,G)}{\partial G}dx=0 \tag{6}$$

3. Inhomogeneity functions of legs materials $\xi_{n,p}$(x) are found from condition:

$$H^*_{n,p}(T(x),q(x),t(x),\psi(x),\xi(x),j,G)\ =\max_{\xi_{n,p}\in U_\xi}H_{n,p}(T(x),q(x),t(x),\psi(x),\xi,j,G) \tag{7}$$

In the case of searching for optimally homogeneous materials, instead of (7) to find the optimal values of the concentration of current carriers in the legs $\xi_{n,p}$, it is necessary to use the relation

$$\begin{gathered}-\frac{\partial J}{\partial \xi_n}+\int_0^1\frac{\partial H_n(\psi,T,q,t,j,G)}{\partial \xi_n}dx=0,\\ -\frac{\partial J}{\partial \xi_p}+\int_0^1\frac{\partial H_p(\psi,T,q,t,j,G)}{\partial \xi_p}dx=0.\end{gathered} \tag{8}$$

Here *H* is the Hamilton-Pontryagin function

$$H_{n,p}=\left(\psi_1f_1+\psi_2f_2\ +\psi_3f_3\ \right)_{n,p}, \tag{9}$$

where $(f_1, f_2, f_3)_{n,p}$ are the right-hand parts of the system of differential equations (1), $\psi = (\psi_1, \psi_2, \psi_3)_{n,p}$ is the momentum vector determined from the solution of the auxiliary system of differential equations canonically conjugate to system (1)

$$\left.\begin{aligned} &\frac{d\psi_1}{dx} = \frac{\alpha\ j}{\kappa}R_1\psi_1 - \left(\frac{\alpha\ j}{\kappa}R_2 - \frac{\alpha_e l}{(S-S_K)\,j}\right)\psi_2 + \frac{\alpha_e}{Gc_P}\psi_3, \\ &\frac{d\psi_2}{dx} = \frac{j}{\kappa}\psi_1 - \frac{\alpha\ j}{\kappa}\psi_2, \\ &\frac{dt}{dx} = -\frac{\alpha_e l}{(S-S_K)\,j}\psi_2 - \frac{\alpha_e}{Gc_P}\psi_3, \end{aligned}\right\}_{n,p} \tag{10}$$

where

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

with the boundary conditions

$$\begin{aligned} &\psi_1^n(1) + \psi_1^p(1) = 0, \qquad \psi_2^n(1) = \psi_2^p(1), \\ &\psi_2^{n,p}(0) = -\frac{\dfrac{j(S-S_K)}{l}}{\sum\limits_{n,p}\left\{Gc_P\left(T_m - t(0)\right) + \left(q(0) + j\dfrac{r_0}{l}\right)\dfrac{j(S-S_K)}{l}\right\}}, \\ &\psi_3^{n,p}(0) = \frac{Gc_P}{\sum\limits_{n,p}\left\{Gc_P\left(T_m - t(0)\right) + \left(q(0) + j\dfrac{r_0}{l}\right)\dfrac{j(S-S_K)}{l}\right\}}. \end{aligned} \tag{11}$$

Based on the system of equations (1), (2), (5) – (11), a computer program has been developed that allows one to determine the optimal distribution of the current carrier concentration $\xi_{n,p}$(x), the heat carrier flow rate G and the electric current density j, whereby the efficiency (3) of the permeable thermoelement will be maximum.

Calculation results of a permeable thermoelement made of materials based on *Bi-Te-Se-Sb*

Let us consider the application of the described method for calculating a permeable thermoelement with a leg height of 1 cm, a cross-sectional area $S - S_K = 1$ cm^2, the temperature of the cold junctions $T_c = 300$ K; the leg materials are solid solutions $Bi_2(TeSe)_3$ of *n*-type conductivity and $(BiSb)_2Te_3$ for a leg of *p*-type conductivity. Fig. 3 shows the temperature and concentration dependences of such materials obtained by approximating experimental data from the literary sources [10].

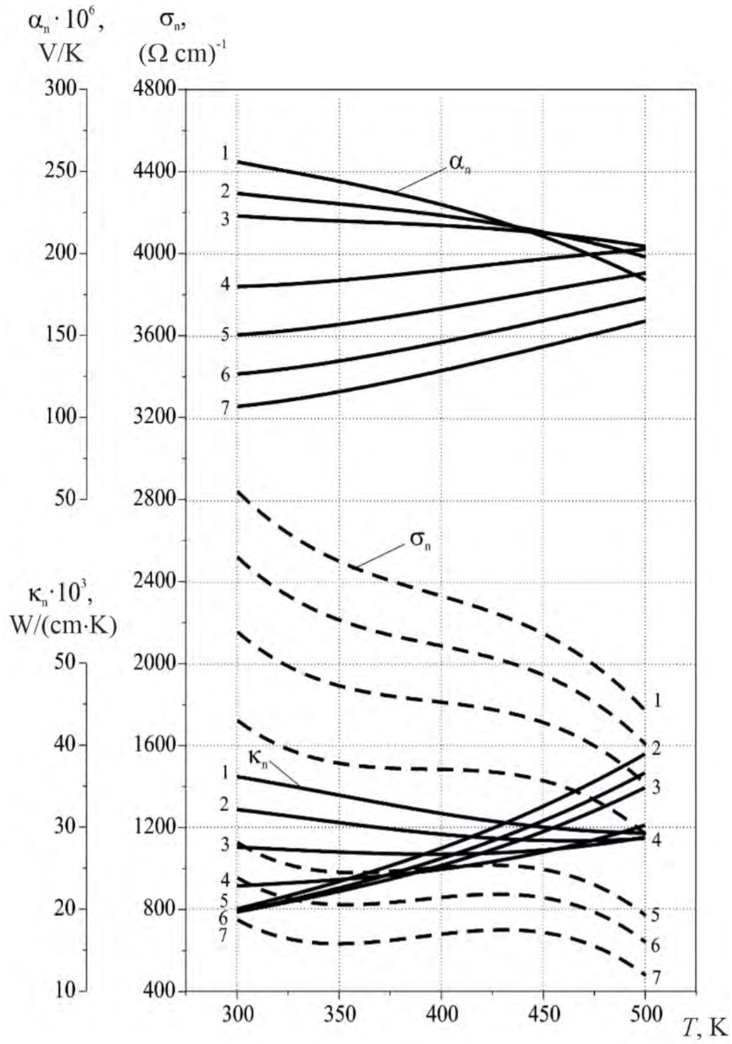

Fig. 2. Temperature dependences of material parameters for different concentrations of current carriers:1 – $6 \cdot 10^{18}$ cm^{-3}, 2 – $8 \cdot 10^{18}$ cm^{-3}, 3 – $1 \cdot 10^{19}$ cm^{-3}, 4 – $2 \cdot 10^{19}$ cm^{-3}, 5 – $3 \cdot 10^{19}$ cm^{-3}, 6 – $4 \cdot 10^{19}$ cm^{-3}, 7 – $5 \cdot 10^{19}$ cm^{-3}.

These materials are most widely used to create thermoelectric elements and modules based on them, operating in the temperature range of 300 – 500 K. The given dependences were used as limitations imposed on the properties of the leg materials during computer calculations.

An example of the optimal FGM distribution for the material of *n*- and *p*-type legs is shown in Fig. 4. With this distribution, volumetric thermoelectric effects are realized in the best way, which gives the maximum value of the efficiency of thermal into electrical energy conversion.

Calculations of the efficiency of permeable thermoelements using functionally graded materials were carried out and the results were compared with the efficiency of a permeable thermoelement made of a homogeneous material. The developed computer design methods make it possible to obtain, as a zero approximation, the efficiency value for a permeable thermoelement made of a homogeneous material, taking into account the temperature dependence of the material properties and the choice of such a value of the current carrier concentration for electrons and holes, at which the best efficiency value is achieved in a given temperature range.

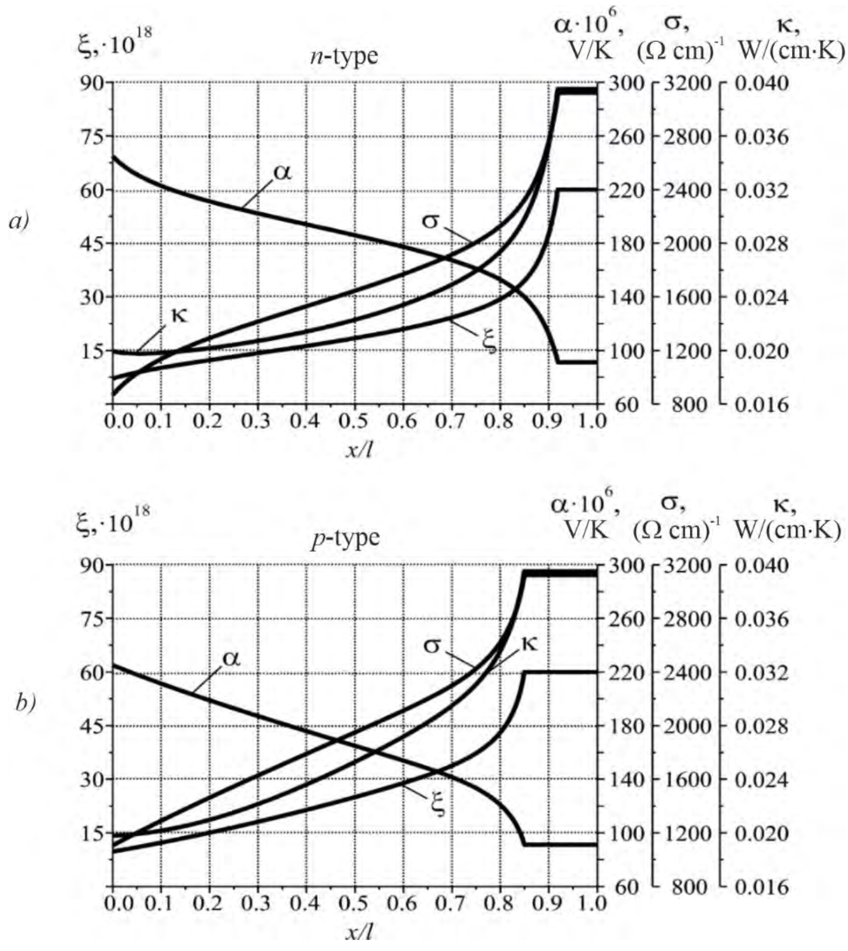

Fig. 3. Optimal distribution of parameters α, σ, κ of a permeable thermoelement along the length of leg l: a) for solid solutions $Bi_2(TeSe)_3$ of n-type conductivity; b) for solid solutions $(BiSb)_2Te_3$ of p-type conductivity; ξ – optimal concentration of current carriers; α, σ, κ – optimal Seebeck coefficient, electrical conductivity and thermal conductivity; heat carrier temperature at the input to thermoelement – 600 K; temperature of thermoelement cold junctions – 300 K; effective heat transfer coefficient – 0.1 W/K.

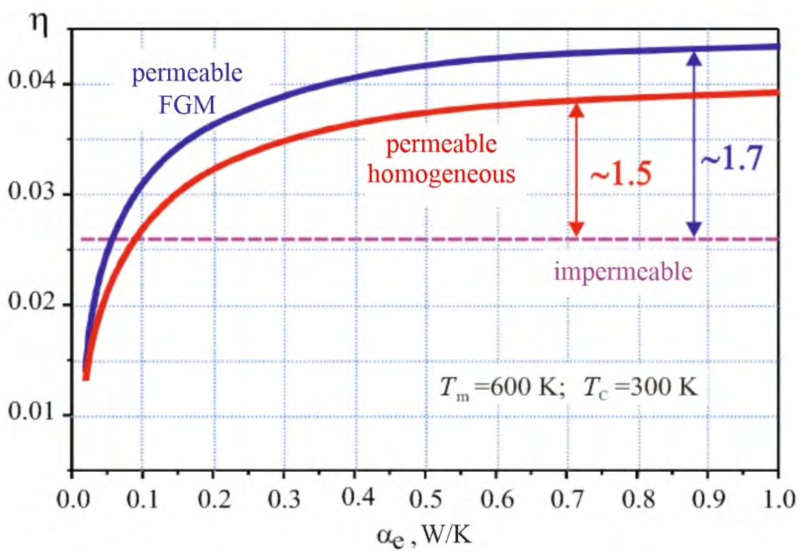

Fig. 4. Dependences of maximum efficiency of a permeable generator thermoelement on the effective coefficient of heat transfer α_e.

Computer studies of the maximum values of energy characteristics (efficiency and power) that are realized at optimal FGM, electric current density and heat carrier pumping speed have been carried out. The results of the obtained efficiency values and their comparison are shown in Fig. 4.

It is evident that the efficiency increases by 1.4 times when using permeable homogeneous thermoelements compared to impermeable ones, and by 1.7 times when using permeable thermoelements made of functionally graded materials.

Conclusions

1. Based on the Pontryagin maximum principle of optimal control theory, a method for computer design of optimal functions of thermoelectric material inhomogeneity for permeable thermoelements of maximum efficiency of thermal into electrical energy conversion has been developed.
2. The method was tested on a model of a thermocouple generator thermoelement with permeable legs for materials based on *Bi-Te-Se-Sb*. Computer methods were used to find the optimal distribution functions of the inhomogeneity of electrical conductivity, thermoEMF and thermal conductivity for *n-* and *p-*type materials.
3. It has been shown that permeable thermoelements made of FGM based on *Bi-Te-Se-Sb* at a heat carrier temperature of 600 K provide an increase in efficiency by 1.4 times, and when using permeable thermoelements made of functionally graded materials – by 1.7 times compared to traditional thermoelements.
4. The results obtained indicate the potential of using optimal control theory methods for designing permeable thermoelements made of FGM.

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КОМП'ЮТЕРНЕ ПРОЕКТУВАННЯ ПРОНИКНИХ ФУНКЦІОНАЛЬНО-ГРАДІЄНТНИХ МАТЕРІАЛІВ ДЛЯ ТЕРМОЕЛЕМЕНТІВ В РЕЖИМІ ГЕНЕРАЦІЇ ЕЛЕКТРИЧНОЇ ЕНЕРГІЇ

На основі принципу максимуму Л.С. Понтрягіна теорії оптимального керування представлено методику проектування оптимальних функціонально-градієнтних матеріалів (ФГМ) для проникних термоелектричних елементів. Створено алгоритм та комп'ютерну програму, яку апробовано для знаходження оптимального ФГМ для віток n- та p- типів провідності на основі Bi-Te-Se-Sb. Показано, що в оптимальних умовах, досягається підвищення ККД при використанні проникних генераторних термоелементів із ФГМ у 1.3 – 1.7 раз порівняно з традиційними термоелементами із однорідних віток.

Ключові слова: комп'ютерне проектування, проникні структури.

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