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Theoretical investigation of permeable segmented generator thermoelement on the base of Bi-Te, Pb-Te, Si-Ge

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Results of computer study on permeable segmented generator thermoelement under efficiency-optimal operating conditions are set forth. Method for solving a multi-parameter optimization problem is described. Heat carrier flow rate, electric current density, parameters of current carrier concentration in each leg segment whereby energy conversion process is maximum thermodynamically efficient are determined. The results of research on a permeable segmented generator thermoelement based on Bi_2Te_3, PbTe, PbTeGe, SiGe, $FeSi_2$ materials are presented. Comparison to conventional thermoelements showed the possibility of efficiency increase by 30 –40% and generated power by 20-30%.

Keywords: generator thermoelement, segmented legs, optimization, efficiency, electric power.

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Introduction

A promising line for thermoelectric element efficiency increase is to use in the legs two or more materials – segments, the thermoelectric properties of which are selected from condition of maximum figure of merit parameter [1]. The elaborated numerical methods for calculation of such thermoelements [2] were used for design of patented in [3, 4] segmented thermoelements using materials based on Bi_2Te_3 and scutterudites. It was theoretically shown [5] that one should expect the efficiency value equal to 15 % with temperature difference about 670 K.

Another promising direction of energy conversion efficiency increase is to use legs permeable to heat carrier flows (liquid or gas) [6]. Due to the presence of heat exchange between heat carrier and “cold” parts of legs it allows to give more thermal energy to material and convert it into electric energy. Computer calculations of such permeable models of thermoelements [7, 8] confirmed the possibility of improving the efficiency of energy conversion by 30%.

The first results of theoretical research on permeable generator thermoelements using segmented legs were given for materials based on Bi_2Te_3 [9]. Method for calculation and optimization of thermoelement operation under maximum efficiency mode at heat carrier pumping velocity and electric current density was described. The effect of structural factors (leg height, channel diameter and number) on the efficiency and electric power was studied. The results showed the possibility of further efficiency increase However, the problem of finding the optimal segmented legs of various materials was not solved.

The purpose of this work is to determine the energy characteristics of a permeable thermoelement of composite legs of different materials under conditions of complex optimization for thermophysical and structural parameters (electric current, heat carrier pumping velocity, number and diameter of channels, leg height).

I. Physical model and its mathematical description

Physical model of permeable segmented thermoelement in electric energy generation mode is shown in Fig. 1. The thermoelement consists of *n*- and *p*-type legs the physical properties of which are temperature-dependent. Heat input is done by passing heat carrier along the leg through the channels (pores). Each leg consists of N_n and N_p segments, respectively, connection contact resistance is r_0, the lateral surfaces of legs are adiabatically insulated, heat carrier temperature at the inlet to thermoelement T_m is assigned. The temperature of cold junctions T_c is thermostated.

A system of differential equations describing the distribution of temperatures and heat flows in a steady-state one-dimensional case in the infinitesimal part dx of each k-th section of n- and p-type legs in dimensionless coordinates is of the form [9]

$$\left.\begin{aligned} \frac{dT}{dx} &= -\frac{\alpha_k j}{\kappa_k} T - \frac{j}{\kappa_k} q, \\ \frac{dq}{dx} &= \frac{\alpha_k^2 j}{\kappa_k} T + \frac{\alpha_k j}{\kappa_k} q + j\rho_k + \frac{\alpha_T P_K^1 N_K l_K^2}{(S-S_K) j}(t-T), \\ \frac{dt}{dx} &= \frac{\alpha_T P_K^1 N_K l_K}{G c_P}(t-T), \end{aligned}\right\} \begin{matrix} k=1,\dots N_{n,p} \\ x_{k-1} \le x \le x_k \end{matrix} \qquad (1)$$

where P_K^1 is channel perimeter; N_K is number of channels; S_K is cross-sectional area of all channels; S is cross-section of leg together with channels; G is heat carrier flow rate in channels; c_p is specific heat of heat carrier; t is temperature of heat carrier at point x; T is temperature of leg at point x; α_T is coefficient of heat transfer; α, κ, ρ are the Seebeck coefficient, thermal conductivity and electric resistivity of leg material.

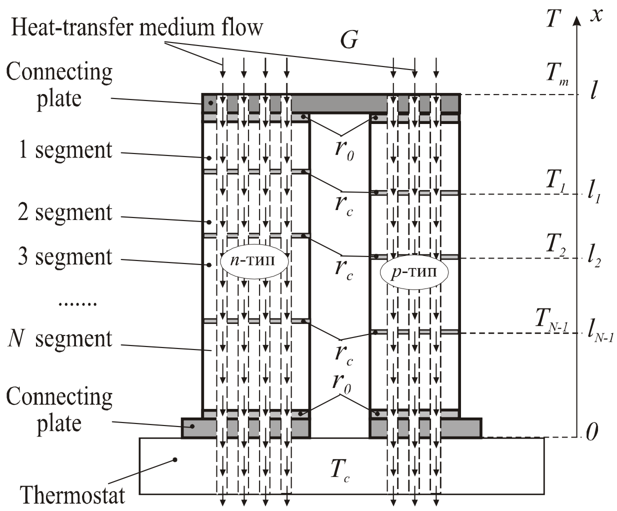


Fig. 1. Physical model of permeable segmented thermoelement.

Specific heat flows q and reduced density of electric current j are determined by relationships

$$q = \frac{Q}{I}, \qquad j = \frac{Il}{S}, \qquad (2)$$

where Q is power of heat flow passing through thermoelement leg, I is electric current, $S_{n,p}$ is cross-sectional area of n- and p-type thermoelement legs.

The boundary conditions necessary for solving (1) with regard to the Joule heat release due to contact resistance r_0 at the junctions of legs will be written as

$$T_{n,p}(0) = T_c, \quad t_{n,p}(1) = T_m, \quad q_{n,p}(1)=0,$$

$$T_{n,p}(x_k^+) = T_{n,p}(x_k^-), \quad q_{n,p}(x_k^+) = q_{n,p}(x_k^-) + \frac{r_0}{S_{n,p}} I, \qquad (3)$$

where indexes "-" and "+" refer to the values of functions immediately to the left and right of segment boundary x_k; $k = 1, \dots, N$ is index that determines the number of leg segment.

In case of designing optimal current carrier concentrations in thermoelement leg segments, one should assign α, κ, ρ as functions of temperature and current carrier concentration (or impurities) C_k for materials: $\alpha_k = \alpha_k(C_k,T)$, $\rho_k = \rho_k(C_k,T)$, $\kappa_k = \kappa_k(C_k,T)$. The purpose of design of permeable segmented generator thermoelement is to determine such matched parameters (reduced current density j in the legs, heat carrier expenditures in channels G, impurity concentrations in each segment material C_k), whereby the thermoelement efficiency achieves maximum value.

The efficiency will be determined through the ratio between thermoelement power and a change in heat carrier enthalpy as follows:

$$\eta = \frac{W}{\sum_{n,p} G c_p (T_m - T_c)} \qquad (4)$$

Efficiency maximum can be conveniently reduced to achieving functional minimum

$$J = \ln\left[\sum_{n,p}\{G c_p (T_m - T_c)\}\right] - \ln\left[\sum_{n,p}\left\{G c_p (T_m - t(0)) + q(0)\frac{j(S-S_k)}{l} - I\left(\frac{r_0}{S_n} + \frac{r_0}{S_p}\right)\right\}\right] \qquad (5)$$

The problem was solved using the Pontryagin maximum principle [10] giving the necessary optimality conditions:

1) optimal values of specific current density in thermoelement legs j should satisfy the equalities

$$-\left[\frac{\partial J}{\partial j}\right]_{n,p} + \sum_{n,p}\int_0^1 \left[\Psi_1^k \frac{\partial f_1^k}{\partial j_k} + \Psi_2^k \frac{\partial f_2^k}{\partial j_k} + \Psi_3^k \frac{\partial f_3^k}{\partial j_k}\right]_{n,p} dx = 0 \qquad (6)$$

where $(f_1^k, f_2^k, f_3^k)_{n,p}$ are right-hand sides of equations (1), $\Psi = (\Psi_1^k, \Psi_2^k, \Psi_3^k)_{n,p}$ is vector-function of pulses [9, 10] which is found from solving the auxiliary system of differential equations

$$\left.\begin{aligned} \frac{d\Psi_1}{dx} &= \frac{\alpha_k j_k}{\kappa_k} R_1 \Psi_1 - \left(\frac{\alpha_k j_k}{\kappa_k} R_2 - \frac{\alpha_e l_k}{(S-S_K) j_k}\right)\Psi_2 + \frac{\alpha_T P_K^1 N_K}{Gc_P}\Psi_3, \\ \frac{d\Psi_2}{dx} &= \frac{j_k}{\kappa_k}\Psi_1 - \frac{\alpha_k j_k}{\kappa_k}\Psi_2, \\ \frac{d\Psi_1}{dx} &= \frac{\alpha_T P_K^1 N_K l_k}{(S-S_K) j_k}\Psi_2 - \frac{\alpha_T P_K^1 N_K}{Gc_P}\Psi_3 \end{aligned}\right\}_{n,p} \tag{7}$$

where

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

with the boundary conditions

$$\begin{aligned} \Psi_1^{n,p}(1) &= 0, \\ \Psi_1^{n,p}(0) &= \frac{\frac{j(S-S_K)}{l}}{\sum_{n,p}\left\{Gc_p\left(T_m - t(0)\right) + q(0)\frac{j(S-S_k)}{l} - I\left(\frac{r_0}{S_n} + \frac{r_0}{S_p}\right)\right\}}, \\ \Psi_3^{n,p}(0) &= \frac{Gc_p}{\sum_{n,p}\left\{Gc_p\left(T_m - t(0)\right) + q(0)\frac{j(S-S_k)}{l} - I\left(\frac{r_0}{S_n} + \frac{r_0}{S_p}\right)\right\}}, \end{aligned} \tag{8}$$

2) optimal values of heat carrier flow rate in channels G

$$-\left[\frac{\partial J}{\partial G}\right]_{n,p} + \sum_{n,p}\int_0^1 \left[\Psi_1^k \frac{\partial f_1^k}{\partial G} + \Psi_2^k \frac{\partial f_2^k}{\partial G} + \Psi_3^k \frac{\partial f_3^k}{\partial G}\right]_{n,p} dx = 0 \tag{9}$$

3) optimal values of impurity concentrations in each segment material C_k are found from the relationships

$$\int_0^1 \left[\Psi_1^k \frac{\partial f_1^k}{\partial C_k} + \Psi_2^k \frac{\partial f_2^k}{\partial C_k} + \Psi_3^k \frac{\partial f_3^k}{\partial C_k}\right]_{n,p} dx = 0\,, k = 1 \ldots, N_{n,p} \tag{10}$$

In case of thermoelement design for fixed materials in segments, the optimality conditions (10) are ignored.

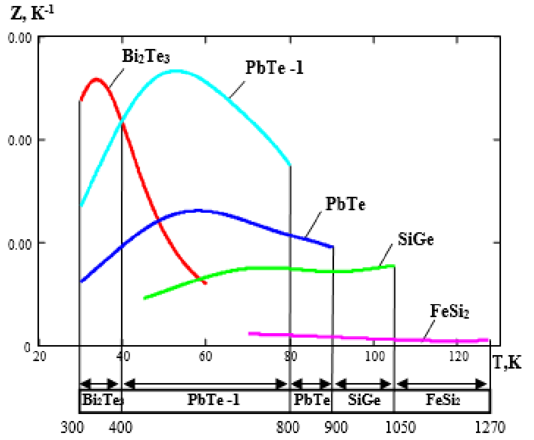
Based on the obtained relationships with the use of successive approximation technique, the Runge-Kutt numerical method for solving a system of differential equations (1) and (7) with the boundary conditions (3) and (8), the Newton method for solving systems of integrally-differential equations (6), (9), (10), a computer program was design of permeable segmented thermoelement was developed. The results of computer study of thermoelement are given below.

II. Results of computer study of the energy characteristics of permeable segmented generator thermoelement

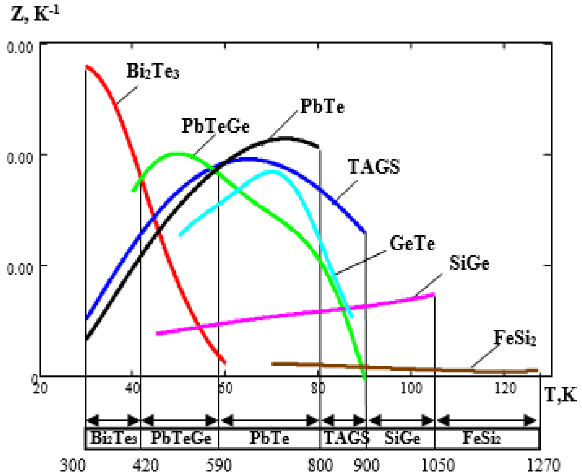
Consider the results of computer simulation of permeable segmented thermoelements based on Bi_2Te_3, *PbTe, SiGe,* $FeSi_2$ materials for *n*-type leg and Bi_2Te_3, *PbTeGe, PbTe, SiGe,* $FeSi_2$ for *p*-type leg. The data on temperature dependences of parameters α, κ, σ of these materials borrowed from the literature sources were approximated by least-squares method with a relative error not more than 0.5% and used for calculation in computer program. Temperature dependences of the figure of merit parameter of these materials are given in Fig.2.

Comparing the figure of merit Z values of the referred materials one can single out the rational areas of temperature (marked in Fig.2) where the use of materials can have maximum effect. Thus, for *n*-type leg maximum figure of merit in the temperature range of 300-400 K is offered by Bi_2Te_3 material, in the temperature range of 400-800 K – by *PbTe-1,* in the temperature range of 800-900 K – by *PbTe,* in the temperature range of 900-1050 K – by *SiGe,* in the temperature range of 1050-1273 K – by $FeSi_2$. It is noteworthy that the figure of merit value for such materials as *PbTe, SiGe* is practically half that for Bi_2Te_3. Therefore, a reply to question whether the increase of temperature difference on a segmented thermoelement will be able to compensate a reduction of total figure of merit of high-temperature materials can be provided only by computer experiment. Computer simulation of permeable segmented thermoelements will also enable determination of the contribution of the bulk Seebeck and Peltier effects arising at connection points of segments to energy conversion efficiency.

Computer simulation of temperature fields in material of thermoelement leg and heat carrier under optimal values of heat carrier flow rate and electric current density was performed. Fig. 3 represents an example of such calculations for the case of five-segmented permeable thermoelement with the legs based on materials shown in Fig.2, general leg height 2 cm, channels of diameter 0.1 cm located at the density of twenty five pcs per 1 cm^2 and cold junction temperature 300 K. It is seen that the use of five-segmented legs is not expedient, since the fourth and fifth segments contribute little (about 40 K) to total temperature difference 450K on thermoelement. From the technological difficulty of creating five-segmented legs it follows that the rational number of segments in this case is three. Similar results were also obtained for *p*-type leg.



a)



b)

Fig. 2. Temperature dependences of figure of merit *Z* of thermoelectric materials.

Dependence of maximum efficiency η and the respective specific electric power *W* of permeable thermoelement at optimal values *j*, *G* on the total height of leg segments l_k is shown in Fig. 4. The plots are given for different number of leg segments *N* (one pcs, two pcs, three pcs and five pcs) at inlet gas temperature 800 K. It can be seen that with increasing height of leg segments, the efficiency grows and reaches saturation close to value 6.2%, and the respective specific power has a pronounced extreme in the field of low values of *l* (0.3cm).

With increasing the number of leg segments, there is a reduction in maximum efficiency values. Thus, the rational number of leg segments is two- three, as long as further increase of segments leads to increasing the number of contact resistances at junction points of leg segments on which the Joule-Lenz parasitic heat is released. This conclusion is also valid for classical segmented thermoelements [11].

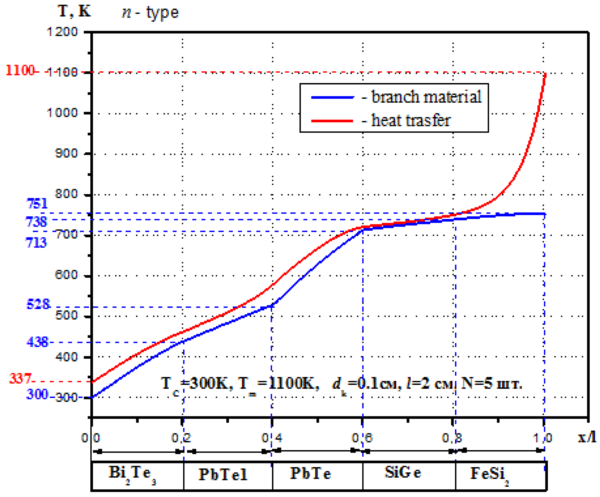


Fig. 3. Temperature distribution in a segmented leg of *n*-type thermoelement.

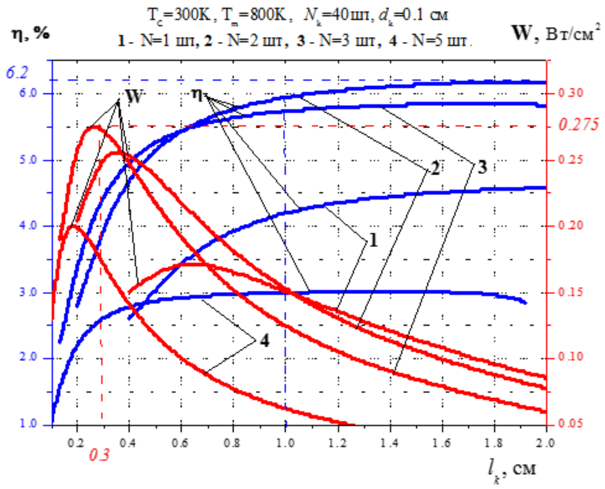


Fig. 4. Energy characteristics of a permeable segmented.

Conclusions

1. A physical model is described, as well as a method of designing a permeable segmented generator thermoelement, where heat carrier is pumped through legs consisting of interconnected segments of various semiconductor materials.
2. For materials based on Bi_2Te_3, *PbTe*, *PbTeGe* *SiGe*, $FeSi_2$ the effect of structural parameters under optimal operating conditions on the energy characteristics of thermoelement was calculated. The rational values of such parameters that enable determination of the necessary material research requirements for creation of thermoelement were revealed.
3. In case of using a permeable segmented thermoelement based on Bi_2Te_3, *PbTe*, *PbTeGe*, *SiGe*, $FeSi_2$ working at the initial heat carrier temperature 800 K and thermostating of cold junctions at 300 K, the rational number of leg segments is two– three. Comparison in thermodynamic efficiency of power conversion to conventional thermoelements showed the possibility of

efficiency increase by 30–40 % and generated power by 20-30%.

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[1] B.W. Swanson, E.V. Somers, R.R. Heikes, J. of Heat Transfer, 83, 77 (1961); https://doi.org/10.1115/1.3680473.
[2] Thermoelectric unicouple used for power generation. Patent 6563039 B2 USA InCl H 01 L 35/28 / Caillat T., Fleurial J.-P., Borshchevsky A., Snyder J., Zoltan A., Zoltan, L. (USA); California Institute of Technology. N 09/765062; Filed 17.01.2001; Publ. 13.05.2003. – 8 p.
[3] Thermoelectric unicouple used for power generation. Patent 6673996 B2 USA InCl H 01 L 35/34 / Caillat T., Zoltan A., Zoltan, L., Snyder J. (USA); California Institute of Technology. N 10/138040; Filed 01.05.2002; Publ. 06.01.2004. – 7 p.
[4] T. Calliat, J.-P. Fleurial, G.J. Snyder, A. Zoltan, D. Zoltan, A. Borshchevsky, Proc. of the XVIIIth International Conf. on Thermoelectrics (USA, 1999), p. 473.
[5] Mohamed S. El-Genk and Hamed H.Saber, Energy Conversion and Management, 44(7), 1069 (2003); https://doi.org/10.1016/S0196-8904(02)00109-7.
[6] Method for improvement of thermoelectric generator efficiency. USSR Certificate of Authorship №162578 / I.V. Zorin, Filed 02.05.1968.
[7] L.I. Anatychuk, R.G.Cherkez, Permeable thermoelement in generation electric energy mod // J.Thermoelectricity, 2, 36 (2003).
[8] L.I. Anatychuk, O.J.Luste, V.Ya.Mikhailovsky, J.Thermoelectricity. Thermoelectric generators for avtomobiles , 4, 21 (2005).
[9] L.I. Anatychuk, R.G.Cherkez, Permeabler segmented thermoelemen in generation mod// J.Thermoelectricity, 3, 5 (2010).
[10] L.S. Pontryagin, V.G. Boltyansky, R.V. Gamkrelidze, E.F. Mischenko, Mathematical Theory of Optimal Processes (Moscow: Nauka, 1976), p.392.
[11] L.I. Anatychuk, L.N. Vikhor, Energy Conversion and Management, 50(9), 2366 (2009); https://doi.org/10.1016/j.enconman.2009.05.020.

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Теоретичні дослідження проникного сегментного генераторного термоелемента на основі Bi-Te, Pb-Te, Si-Ge

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Наведено результати комп'ютерного дослідження проникного сегментованого термоелемента генератора в умовах оптимальної ефективності роботи. Описано метод розв'язання багатопараметрічної оптимізаційної задачі. Визначено швидкість потоку теплоносія, густину електричного струму, параметри концентрації носіїв струму в кожному сегменті, при якому процес перетворення енергії є максимально термодинамічно ефективним. Наведено результати досліджень проникного сегментованого генераторного термоелемента на основі матеріалів Bi-Te, Pb-Te, PbTeGe, Si-Ge. Порівняння зі звичайними термоелементами показало можливість збільшення ККД на 30-40% і виробленої потужності на 20-30%.

Ключові слова: генераторний термоелемент, сегментовані елементи, оптимізація, ефективність, електрична потужність.