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MODELING OF THERMOELECTRIC CONVERTER CHARACTERISTICS

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Under the rough estimation the annual worldwide production of thermoelectric converters (modules) for the needs of thermoelectric power generation and cooling reaches more than 50 million pieces. The thermoelectric convertors are mechanically stable, high-reliable with a life cycle up to 20 years. The main disadvantage is their low energy efficiency. This especially applies to miniature modules with a length of thermoelements in the range from 500 μm down to 200 μm. Their low efficiency is due to the effect of electrical and thermal resistances of contacts, interconnectors and insulating plates. One way to improve the efficiency of thermoelectric generators and coolers is to optimize the materials and structure of thermoelectric modules for the required operating conditions. For this purpose, it is advisable to use methods of optimal control theory. They are suitable for optimizing single- and multi-stage converters made of homogeneous or inhomogeneous, so-called functionally graded thermoelectric materials (FGTM). The optimal control method makes it possible to take into consideration the temperature dependences of the thermoelectric parameters of materials, additional bulk thermoelectric effects that occur in FGTMs, and the influence of unwanted electrical and thermal resistances in modules. This lecture outlines the main concepts of the optimal control theory and explains how to use them to design modules with optimal structure and simulate module characteristics. Examples of modeling the convertor performances are considered and the effect of undesirable electrical and thermal resistances on the maximum efficiency of cooling and generating converters made of Bi_2Te_3*-based materials is analyzed. It is shown that the efficiency of modules, especially of miniature ones, can be significantly improved if these unwanted resistances are reduced to their rational values. The decrease in electrical contact resistance is the predominant factor. The rational values to which it is advisable to decrease the electrical contact resistivity have been determined. It is necessary to focus on such rational contact resistance values in the development of modules' technology. Bibl. 9, Figs. 9, Tabl. 2.*

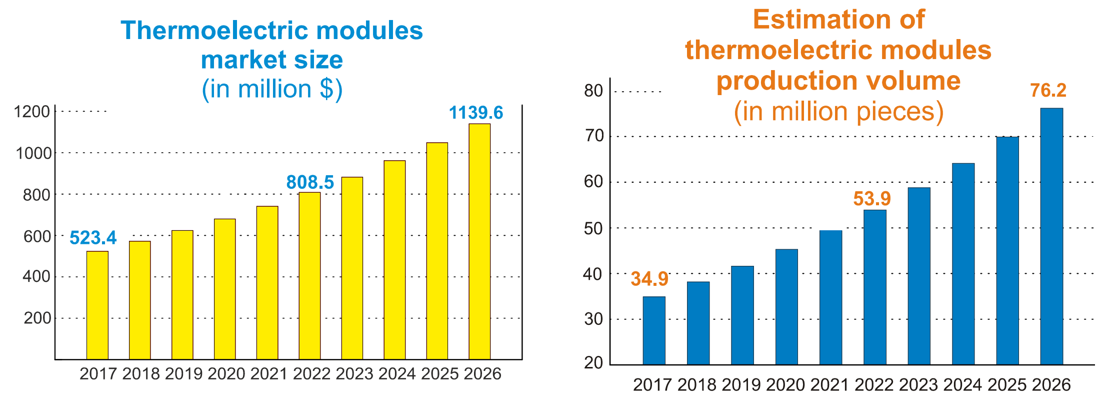
Key words: thermoelectric converter, thermoelectric module efficiency, methods of optimal control theory, coefficient of performance, electrical contact resistance, thermal resistance of interconnect and insulating plates.

Introduction

It is well known that thermoelectric (TE) convertors (usually we call them modules) have a lot of important applications. Thermoelectric devices are widely used for cooling, controlling thermal conditions and stabilizing the temperature of electronic elements and systems, such as various sensors, laser diodes, light emitting diodes, computer chips and so on [1].

TE generators are used in applications where a heat source exists. In some cases, they can even replace batteries, for example to power wireless sensors for monitoring the operating condition of industrial processes or of pipelines [2]. TE converters are used in nuclear-based small-scale power sources for space or biomedical applications [3]. Miniscale TE generators that use human body heat, are the promising energy sources for wearable electronics [4].

Fig. 1a shows a diagram of the growth in the market size of thermoelectric modules. The market compound annual growth rate (CAGR) is about 9 %. Using this diagram and assuming that the average price of a standard TE module is near $15, we can easily estimate the annual production of modules in the world [5]. The results of such rough estimation are shown in Fig.1b. It is seen that now production reaches more than 50 million pieces per year.



a) *b)*

Fig. 1. World market size (a) and estimation of production volume (b) of thermoelectric modules

The thermoelectric convertors are mechanically stable, high-reliable with a life cycle up to 20 years. The main disadvantage is their low energy efficiency.

Ideal model for module optimization

One way to improve the efficiency of thermoelectric generators and coolers is to optimize the materials and structure of thermoelectric modules for the required operating conditions. In the 50s of last century A. Ioffe with colleagues got the main optimal relations for an ideal thermocouple of homogeneous materials with temperature-independent properties [6]. These relationships are still used today as the simplest method for designing the cooling and generating modules and calculating their performance.

Simple modeling of cooling modules

Let's consider these relationships for the cooling module. Fig. 2 shows a thermocouple for modules in cooling mode.

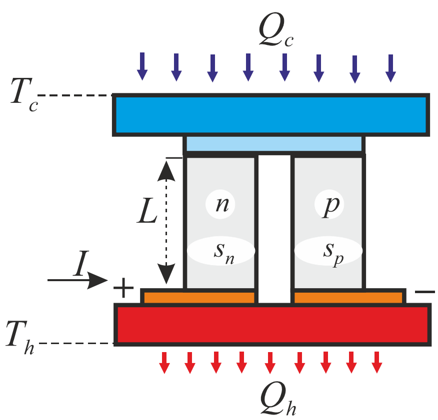


Fig. 2. Schematic of ideal thermocouple for modules in cooling mode

The module contains a number of thermocouples made of semiconductor n- and p-type legs, which are commonly referred as thermoelements. If we pass an electric current I with the polarity indicated in Fig. 2 and maintain the heat-liberating surface of the module at a temperature of T_h close to the ambient temperature, then the heat-absorbing surface will be cooled to a certain temperature of T_c. The module will operate in cooling mode.

Energy balance equations for a thermocouple which are used for optimization have the form

$$\begin{aligned} Q_c &= \alpha T_c I - \frac{1}{2} I^2 R - K\Delta T \\ Q_h &= \alpha T_h I + \frac{1}{2} I^2 R - K\Delta T \end{aligned}, \tag{1}$$

where $\alpha = \alpha_p + |\alpha_n|$, $R = L(\rho_p / s_p + \rho_n / s_n)$, $K = (\kappa_p s_p + \kappa_n s_n)/L$.

The energy efficiency of the module is estimated by the coefficient of performance:

$$\mathrm{COP} = \frac{Q_c}{W} = \frac{Q_c}{Q_h - Q_c}, \tag{2}$$

where Q_c is the cooling capacity, W is the consumed electrical power, Q_h is the amount of heat given to the ambient.

The design of the module, as a rule, is carried out for the maximum COP mode for a given temperature difference.

Balance equations (1) are used for multi-parameter optimization and determination of the maximum COP value under the conditions of given T_c, T_h. As a result, the following expressions are obtained for calculating the optimal values of parameters, such as the ratio of cross section areas of the thermocouple legs

$$\left(s_n / s_p\right)_{\mathrm{opt}} = \sqrt{\kappa_n \rho_p} \Big/ \sqrt{\kappa_p \rho_n} \tag{3}$$

and optimal current value

$$\left(I\right)_{\mathrm{opt}\,\varepsilon} = \frac{\alpha \Delta T}{R(M-1)}, \tag{4}$$

where $M = \sqrt{1 + Z_{TE}\overline{T}}$, $\overline{T} = \frac{T_c + T_h}{2}$, $Z_{TE} = \frac{\alpha^2}{\left(\sqrt{\rho_p \kappa_p} + \sqrt{\rho_n \kappa_n}\right)^2}$ is the figure of merit for a thermocouple. If the material parameters of the legs are the same it will be the material figure of merit $Z_{TE} = Z = \frac{\alpha^2}{\rho\kappa}$. A maximum COP is calculated by the formula:

$$\mathrm{COP}_{\max} = \frac{T_c}{\Delta T} \frac{M - T_h / T_c}{M + 1}. \tag{5}$$

In the case of a cascade module, optimal values of inter-stage temperatures T_i are added to the optimal parameters that ensure the maximum value of the COP. They are determined by the approximate relations:

$$T_i = T_c \left(\frac{T_h}{T_c}\right)^{\frac{i}{N}}, \; i = 1, 2, \ldots, N-1, \tag{6}$$

where N is a number of stages. Then the formulas for one-stage module are used for modeling the structure of every stage.

Described method is used for designing of cooling module with the maximum COP at a given temperatures T_c and T_h. For a given value of operating current I, the optimal ratios L/s_n, L/s_p are calculated using the formulas (3) and (4) and the number of thermocouples providing the required cooling capacity Q_m of module is determined as follows $n = Q_m/Q_c$. For a cascade module the ratios $n_i/n_{i+1} = Q_{ci+1}/Q_{hi}$ are used to find the number of thermocouples in every stage. Then module characteristics such as COP_{max}, and the dependences of cooling capacity and supply power or voltage on temperature drop and current are calculated using the formulas (1)-(5).

Simple modeling of generating modules

Fig. 3 shows the thermocouple for generating module. If the absorbing junction is heated by a heat flow Q_h (Fig. 3) to a temperature of T_h, and the opposite junction is maintained at a temperature of T_c by removing of heat Q_c, then due to the Seebeck effect, a thermoEMF appears in a circuit. If the circuit is closed, the electric current passes and a power is generated at the external load R_L. The module operates as a generator.

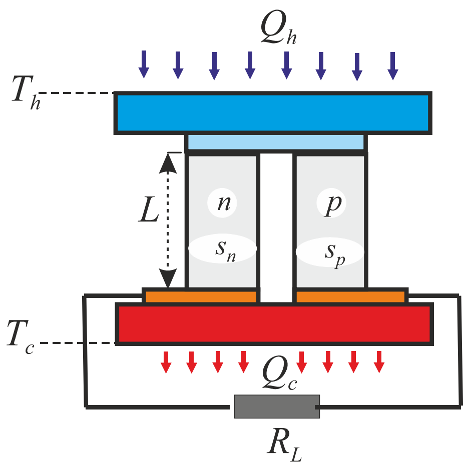


Fig. 3. Schematic of ideal thermocouple for modules in generating mode

Energy balance equations for a thermocouple which are used for optimization have the form

$$\begin{aligned} Q_h &= \alpha T_h I - \frac{1}{2} I^2 R + K\Delta T \\ Q_c &= \alpha T_c I + \frac{1}{2} I^2 R + K\Delta T \end{aligned} . \tag{7}$$

The efficiency is defined as

$$\eta = \frac{W}{Q_h} , \tag{8}$$

where generating power is determined by the formula

$$W = Q_h - Q_c = \alpha I \Delta T - \frac{1}{2} I^2 R . \tag{9}$$

Optimization gives the expression (3) for optimal ratio of legs cross-section areas which is the same as for cooling thermocouple, and the formula for optimal current in a circuit in the form:

$$I_{\text{opt}\,\eta} = \frac{\alpha \Delta T}{R(M+1)} \,. \tag{10}$$

Maximum efficiency, output voltage and power in this mode are calculated as follows

$$\eta_{\max} = \frac{\Delta T}{T_h} \frac{M-1}{M + T_c / T_h} \;,\; V_\eta = \alpha \Delta T - IR = \frac{\alpha \Delta T M}{M+1} \;,\; W_\eta = \frac{\alpha^2 \Delta T M}{R(M+1)^2} \;. \tag{11}$$

It should be mentioned that output voltage and power are close to their maximum values, which occur when load and thermocouple resistances are equal: $R_L = R$. In this case M=1 and the formulas

$$V_{\max} = \alpha \Delta T / 2 \;,\; W_{\max} = \alpha^2 \Delta T / 4R \;,\; I_{\text{opt}\,W} = \alpha \Delta T / 2R \tag{12}$$

are used.

The initial data for designing a generating module are temperatures T_h, T_c, the required electric power W_L and voltage V_L on the external load. Therefore, the current I in the closed circuit is also given and is equal to $I = W_L / V_L$. The optimal cross-sectional areas of the *n*- and *p*-type legs are calculated using the formulas for current $I_{\text{opt}\,\eta}$ or $I_{\text{opt W}}$ and the number of thermocouples providing the required power W_L is determined as $n = W_L / W$.

So, in accordance with the Ioffe formulas (5) and (11) for ideal module model the maximum COP and efficiency are determined by the dimensionless figure of merit ZT of thermoelectric materials for module legs. The ideal model of a TE converter does not take into consideration the following basic physical factors:

- dependence of parameters of TE materials on temperature,
- influence of the Thomson effect,
- influence of electrical and thermal losses in the module structure, namely
  - ✓ influence of contact resistance,
  - ✓ electrical and thermal resistance of connectors,
  - ✓ thermal resistance of insulating plates,
  - ✓ thermal resistance of heat sink on the cold and hot surfaces of module,
- possibility to use inhomogeneous materials for legs.

These factors can significantly affect the characteristics of the TE converter. The optimal structure of the module depends on them. It is shown in [7], how the influence of some factors is approximately taken into consideration if formulas for an ideal module model are used. For example, to take into account the temperature dependences of TE material parameters, their average values

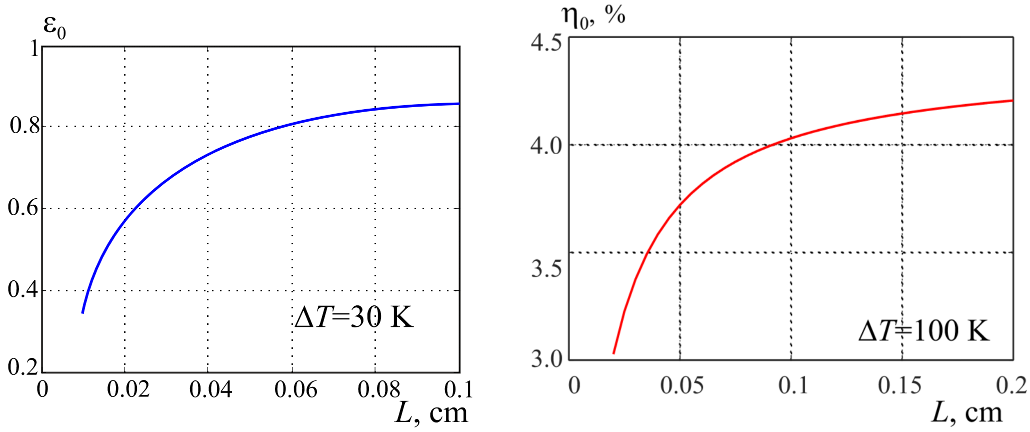
$$\bar{\alpha} = \frac{1}{T_h - T_c} \int_{T_c}^{T_h} \alpha(T) dT \;,\; \bar{\rho} = \frac{1}{T_h - T_c} \int_{T_c}^{T_h} \rho(T) dT \;,\; \bar{\kappa} = \frac{1}{T_h - T_c} \int_{T_c}^{T_h} \kappa(T) dT \tag{13}$$

can be used.

The electrical resistance of contacts at the boundaries between the legs and metal connecting layers is considered as follows

$$\rho = \rho_{\text{mat}} + \frac{2 r_c}{L} \,, \tag{14}$$

where r_c is the contact resistance. In this case the convertor efficiency depends on a leg length as can be seen in Fig. 4.



a) *b)*

Fig. 4. Dependences of maximum COP ε_0 (a) and maximum efficiency η_0 (b) on a thermoelement length L for contact resistivity $r_c = 5\times10^{-6}\ \Omega\,cm^2$

The Joule heat, which is produced on the contacts, reduces the efficiency. A contact resistance is one of the main reasons why Z of materials is not fully realized in thermoelectric coolers and generators.

Methods of optimal control theory for module optimization

To consider all the factors mentioned above, we use a more realistic model of TE convertor and apply methods of optimal control theory for optimization and modeling of module structure and estimation of its performances [8].

A schematic of a TE module for cooling or power generation is shown in Fig. 5.

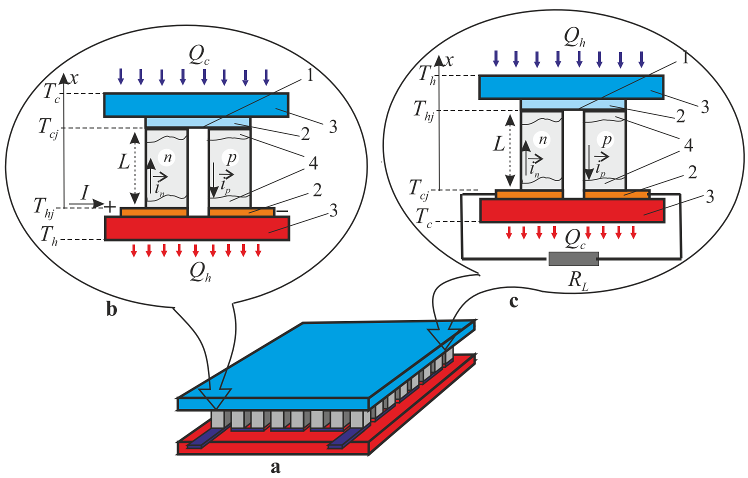


Fig. 5. Schematic of TE module (a) for cooling (b) or power generation (c). 1 – heat-absorbing thermocouple junction, 2 – metallic interconnector, 3 – insulating plate, 4 – contact zone.

Typically, the legs are connected in a series electrical circuit by metallic interconnectors and mounted between two insulating plates in parallel with respect to the heat flow. In general case, the multistage modules can be used for coolers or generators.

This schematic diagram is used to establish the appropriate mathematical relationships for the module physical model. For simplicity, the heat flow is assumed to be one-dimensional. This assumption is reasonable, since the interconnectors and insulating plates are usually thin and made of materials with good thermal conductivity. Therefore, the heat flow along the module surfaces due to local temperature gradients is neglected as it is usually compared to the heat flux across the thermoelements. The heat losses from the edges of the thermoelements and insulating plates are also neglected. Moreover, as shown, for example, in [9], the results of calculating the module parameters using the 3D approach little differ from the results obtained based on the one-dimensional approximation.

To apply methods of optimal control theory, we need to write a system of the first order differential equations for the temperature and heat flux distribution in the TE legs. For this we use the one-dimensional second order equation of heat flow in thermoelectric leg at a steady state, which has the following form

$$\frac{\mathrm{d}}{\mathrm{d}x}\kappa\frac{\mathrm{d}T}{\mathrm{d}x}+\frac{i^2}{\sigma}-T\frac{\mathrm{d}\alpha}{\mathrm{d}T}i\frac{\mathrm{d}T}{\mathrm{d}x}-\frac{\mathrm{d}\alpha}{\mathrm{d}x}iT=0, \tag{15}$$

where $i\equiv\left|\vec{i}\right|=I/s$ is current density. In this equation, the thermoelectric material properties are temperature and coordinate dependent. The third term of Eq. (15) represents the Thomson effect, the last term is the volumetric Peltier effect. To calculate the temperature $T(x)$ and heat flux $q(x)$ distributions in the n- and p-type legs of thermocouple, a new variable $\bar{q}=-\kappa\frac{\mathrm{d}T}{\mathrm{d}x}+\alpha iT$ is used to write the two second order differential equations (15) for n- and p-legs of N-stage module in the form of a system of first order equations as follows

$$\left.\begin{aligned}\frac{dT}{dx}&=-\frac{\alpha i_k}{\kappa}T-\frac{\bar{q}}{\kappa}\\ \frac{d\bar{q}}{dx}&=\frac{\alpha^2 i_k^2}{\kappa}T+\frac{\alpha i_k}{\kappa}\bar{q}+\frac{i_k^2}{\sigma}\end{aligned}\right\}_{n,p}\quad \begin{aligned}&x_{k-1}\le x\le x_k\\ &k=1,\ldots,N\end{aligned}, \tag{16}$$

where we use the equalities $\alpha_n=\left|\alpha_n\right|$ and $\alpha\vec{i}=-\left|\alpha i\right|$ which are true for both n- and p-type legs, since a change in the type of conductivity in a thermocouple occurs simultaneously with a change in the direction of the current density vector. The material characteristics depend on inhomogeneity functions $C_{k\,n,p}(x)$ and temperature, i.e. $\alpha_{k\,n,p}=\alpha_{k\,n,p}\left(C_{k\,n,p}(x),T\right)$, $\sigma_{k\,n,p}=\sigma_{k\,n,p}\left(C_{k\,n,p}(x),T\right)$, $\kappa_{k\,n,p}=\kappa_{k\,n,p}\left(C_{k\,n,p}(x),T\right)$. The functions $C_{k\,n,p}(x)$ characterize the charge carrier concentration distribution in a semiconductor along the height of thermoelement legs, or distribution of impurity concentration or a change in composition of the basic components of thermoelectric material.

To use optimal control methods, it is convenient to rewrite the system (16) taking the specific value of heat flux density $q=Q/I\equiv\bar{q}/i$, dimensionless coordinate $x=x/L$, $0\le x\le L$ and specific value of current density $j_k=i_kL$. The system (16) will take the form

$$\left.\begin{aligned}\frac{dT}{dx}&=-\frac{\alpha j_k}{\kappa}T-\frac{j_k}{\kappa}q,\\ \frac{dq}{dx}&=\frac{\alpha^2 j_k}{\kappa}T+\frac{\alpha j_k}{\kappa}q+\frac{j_k}{\sigma},\end{aligned}\right\}_{n,p}\quad k=1,\ldots,N. \tag{17}$$

The system is suitable for both cooling and generating modes.

Optimal control problem for cooling module

The main input data for designing a module are the cooling temperature T_c, the number of stages N, the temperature of cooler base T_h, and the cooling capacity Q_c. The temperature and inhomogeneity dependences of material properties should be known. The following parameters should also be specified: specific values of contact resistance r_c, electrical and thermal resistances of interconnectors and insulating plates, as well as their thickness, thermal resistances of heat sinks on the hot and cold sides of a module. Usually, the thermoelement length L and the supply current I are given.

The main requirement is the maximum of the COP $\varepsilon = Q_c / W$, where $W = Q_h - Q_c$ is the consumed power. Q_c and Q_h are the absorbed and liberated heat powers.

This problem is equivalent to determining of minimum of a functional

$$J = \ln\frac{Q_h}{Q_c} = \ln\prod_{k=1}^{N}\frac{Q_{1k}}{Q_{0k}} = \ln\prod_{k=1}^{N}\frac{q_{1k}}{q_{0k}} = \sum_{k=1}^{N}(\ln q_{1k} - \ln q_{0k}) \ , \tag{18}$$

where conditions of heat balance between the stages and on the hot and cold module sides in a form

$$\begin{aligned} &Q_{1k+1} = Q_{0k}, \quad k = 1,\dots,N-1, \\ &Q_{11} = -Q_h, \quad Q_{0N} = -Q_c, \end{aligned} \tag{19}$$

and specific heat fluxes on thermocouple junctions in a form

$$q_{1k} = \frac{Q_{1k}}{n_k I}, \quad q_{0k} = \frac{Q_{0k}}{n_k I} \tag{20}$$

were used. These specific heat fluxes are determined by solving the system (17) with the boundary conditions

$$\begin{aligned} &T_{nk}(0) = T_{pk}(0) \equiv T_k(0),\ T_{nk}(1) = T_{pk}(1) \equiv T_k(1),\ k = 1,\dots,N \\ &T_1(0) = T_h + \delta T_0,\ T_N(1) = T_c - \delta T_N,\ T_k(0) = T_{k-1}(1) + \delta T_{k-1},\ k = 2,\dots,N \end{aligned} \tag{21}$$

and using the expressions

$$q_{0\,k} = \sum_{n,p}\left[q_k(1) + j_k\frac{r_c}{L}\right]_{n,p} + q_{con}, \quad q_{1k} = \sum_{n,p}\left[q_k(0) - j_k\frac{r_c}{L}\right]_{n,p} - q_{con}\ , \tag{22}$$

where $q_{con} = \dfrac{2r_{con}I}{l_{con}}\left(K_{con} - \dfrac{2}{3}\right)$. Formulas (22) take into account the release of the Joule heat due to the resistances of contacts r_c and interconnectors r_{con}. In (21), δT is a temperature difference due to the thermal resistances of interconnectors, insulating plates and heat sinks on the hot and cold sides. In a one-dimensional approximation it is calculated as follows

$$\begin{aligned} &\delta T_0 = Q_h(R_{ins} + R_{con} + R_{hs}) = -\frac{q_{11}}{\left(L/(j_1)_n + L/(j_1)_p\right)}R_{th}\,, \\ &\delta T_N = Q_c(R_{ins} + R_{con} + R_{cs}) = -\frac{q_{0N}}{\left(L/(j_N)_n + L/(j_N)_p\right)}R_{tc}\,, \\ &\delta T_k = Q_{0k}(R_{ins} + R_{con}) = -\frac{q_{0k}}{\left(L/(j_k)_n + L/(j_k)_p\right)}R_{tk}\,, k = 1,\dots,N-1\,, \end{aligned} \tag{23}$$

where $R_{th}=\dfrac{l_{con}}{\kappa_{con}K_{con}}+\dfrac{l_{ins}}{\kappa_{ins}K_{ins}}+\dfrac{1}{h_hK_{hs}}$, $R_{tc}=\dfrac{l_{con}}{\kappa_{con}K_{con}}+\dfrac{l_{ins}}{\kappa_{ins}K_{ins}}+\dfrac{1}{h_cK_{cs}}$, $R_{tk}=\dfrac{l_{con}}{\kappa_{con}K_{con}}+\dfrac{l_{ins}}{\kappa_{ins}K_{ins}}$,

κ, l, h, K, are heat conductivity, height, heat transfer coefficients and fill factors of interconnector, insulating plate and heat sinks, respectively.

Optimal control problem for generating module

In this case the initial data for optimization includes the temperatures of the heat-absorbing surface T_h and heat-releasing surface T_c. As a rule, generator module design is made for the assigned values of electrical power W and output voltage V. The value of current is also known and is equal to $I=W/V$.

The efficiency of generating module is defined as the ratio $\eta=\dfrac{W}{Q_h}\equiv\dfrac{Q_h-Q_c}{Q_h}$. Instead of the maximum efficiency we determine the minimum of functional

$$J=\sum_{k=1}^{N}(\ln q_{0k}-\ln q_{1k}) \ . \tag{24}$$

The specific heat fluxes are determined by solving the system (17) with the boundary conditions

$$\begin{gathered} T_{nk}(0)=T_{pk}(0)\equiv T_k(0),\ T_{nk}(1)=T_{pk}(1)\equiv T_k(1),\ k=1,...,N \\ T_1(0)=T_c+\delta T_0,\ T_N(1)=T_h-\delta T_N,\ T_k(0)=T_{k-1}(1)+\delta T_{k-1},\ k=2,...,N \end{gathered} . \tag{25}$$

The expressions for specific heat flux densities have the form

$$q_{1k}=\sum_{n,p}\left[q_k(1)+j_k\frac{r_c}{L}\right]_{n,p}+q_{con},\quad q_{0k}=\sum_{n,p}\left[q_k(0)-j_k\frac{r_c}{L}\right]_{n,p}-q_{con} \ . \tag{26}$$

δT is calculated as follows

$$\delta T_0=Q_h(R_{ins}+R_{con}+R_{hs})=-\frac{q_{11}}{\left(L/(j_1)_n+L/(j_1)_p\right)}R_{th},$$

$$\delta T_N=Q_c(R_{ins}+R_{con}+R_{cs})=-\frac{q_{0N}}{\left(L/(j_N)_n+L/(j_N)_p\right)}R_{tc}, \tag{27}$$

$$\delta T_k=Q_{0k}(R_{ins}+R_{con})=-\frac{q_{0k}}{\left(L/(j_k)_n+L/(j_k)_p\right)}R_{tk},k=1,...,N-1 \ .$$

Optimization problem solution

The efficiency and COP depend of inhomogeneity functions $C_{k\,n,p}(x)$ and current densities$(j_k)_{n,p}$. The problem is to find these optimal functions and these optimal parameters that satisfy the maximum efficiency or COP values. In case of a cascade module, the interstage temperatures should be optimal as well.

According to optimal control theory, for each continuity part of functions T and q the Hamiltonian function is introduced

$$H_k=(\psi_1 f_{1k}+\psi_2 f_{2k}),\qquad k=1,...,N \ . \tag{28}$$

where ($f_{1\,k}$, $f_{2\,k}$) are the right-hand sides of equations (17). $\Psi = (\Psi_1, \Psi_2)$ is a costate vector-function, which is built according to the rule

$$\frac{\partial\psi_1}{\partial x} = -\frac{\partial H}{\partial T},\ \frac{\partial\psi_2}{\partial x} = -\frac{\partial H}{\partial q} \tag{29}$$

and in our case satisfies a system of equations

$$\left.\begin{aligned} \frac{d\psi_1}{dx} &= \frac{\alpha j_k}{\kappa}R_{1k}\psi_1 - \frac{\alpha^2 j_k}{\kappa}R_{2k}\psi_2, \\ \frac{d\psi_2}{dx} &= \frac{j_k}{\kappa}\psi_1 - \frac{\alpha j_k}{\kappa}\psi_2, \end{aligned}\right\}_{n,p} \quad k = 1,\ldots,N\,. \tag{30}$$

where $\left.\begin{aligned} R_{1k} &= 1 + \frac{d\ln\alpha}{dT}T - \frac{d\ln\kappa}{dT}\left(T + \frac{q}{\alpha}\right) \\ R_{2k} &= R_{1k} - \frac{1}{Z}\frac{d\ln\sigma}{dT} + \frac{d\ln\kappa}{dT}\left(T + \frac{q}{\alpha}\right) \end{aligned}\right\}$, $Z = \dfrac{\alpha^2\sigma}{\kappa}$. The boundary conditions for this system are as follows:

for cooling mode

$$\psi_{2(k)_{n,p}}(0) = \frac{1}{q_{1k}},\ \psi_{2(k)_{n,p}}(1) = \frac{1}{q_{0k}} \tag{31}$$

for generating mode

$$\psi_{2(k)_{n,p}}(0) = \frac{1}{q_{0k}},\ \psi_{2(k)_{n,p}}(1) = \frac{1}{q_{1k}} \tag{32}$$

Optimality conditions

According to the optimal control theory, the following conditions must be met for the minimum J:

1. Optimal functions which characterize the inhomogeneity of *n*- and *p*-type thermoelectric materials $C_{k\,n,p}(x)$ must satisfy the Pontryagin maximum principle, namely the condition of the Hamiltonian function maximum

$$H_{k\,n,p}(\psi(x),T(x),q(x),C(x),j) = \max_{C\in G_C} H_{k\,n,p}(\psi(x),T(x),q(x),C,j). \tag{33}$$

2. Optimal current densities in stages are found from the relationships

$$-\frac{\partial J}{\partial(j_k)_{n,p}} + \int_0^1 \frac{\partial H_{k\,n,p}(\psi,T,q,C,(j_k)_{n,p})}{\partial(j_k)_{n,p}}dx = 0 \tag{34}$$

3. The interstage temperatures T_k must satisfy the system of equations

$$\sum_{n,p}\psi_{1(k+1)_{n,p}}(0) = \sum_{n,p}\psi_{1(k)_{n,p}}(1),\quad k = 1,\ \ldots,N-1 \tag{35}$$

Calculation of module structure

The optimal parameters of module structure are calculated according to the following formulas:

- cooling module:

The cross-section of thermoelements and the number of thermocouples in stages are determined as follows $\left(s_k\right)_{n,p} = IL/\left(j_k\right)_{n,p}$, $n_N = -Q_0/q_{0N}I$, $n_k = n_{k+1}\, q_{1k+1}/q_{0k}$, $k = 1,\ldots,N-1$.

The coefficient of performance is calculated using the expression $\varepsilon_{\max} = \dfrac{1}{\exp\left(J_{\min}\right)-1}$.

The electric power required for each stage and module as a whole is found from the relations $W_k = -n_k I\left(q_{1k} - q_{0k}\right)$, $W = \dfrac{Q_0}{\varepsilon}$.

- generating module:

The maximum module efficiency is calculated using the formula $\eta_{\max} = 1 - \exp(J_{\min})$.

The formula for the leg cross-section area is the same as for cooling module.

The optimal number of thermocouples n_k in the stages is determined from the conditions of their thermal compatibility as follows $n_N = -Q_h/q_{1N}I$, $n_k = n_{k+1}\, q_{0k+1}/q_{1k}$, $k = 1,\ldots,N-1$, where the thermal power required for generation of specified electrical power W is determined as the ratio $Q_h = \dfrac{W}{\eta}$.

Iteration algorithm

The problem is solved by a numerical method. The following iteration algorithm is used.

1. At first there are assigned some initial approximations of material inhomogeneity functions $C^{(0)}_{k\, n,p}\left(x\right)$, current densities $\left(j_k\right)^{(0)}_{n,p}$ and the initial distribution of interstage temperatures $T^{(0)}_k$.
2. The main boundary problem with the system (17) is solved. The initial distributions $T^{(0)}_{k\,n,p}\left(x\right)$, $q^{(0)}_{k\,n,p}\left(x\right)$ are found for all the stages and the value of functional $J^{(0)}$ is calculated.
3. The obtained data is used for integration of adjoint equations system (30). We get functions $\Psi_{1(k)n,p}\left(x\right)$, $\Psi_{2(k)n,p}\left(x\right)$.
4. New approximations are found for the inhomogeneity functions $C^{(1)}_{k\, n,p}\left(x\right)$ from the Pontryagin maximum principle (33).
5. The nonlinear systems for current densities (34) and interstage temperatures (35) are solved by the Newton iterations method and new values of current density $\left(j_k\right)^{(1)}_{n,p}$ and interstage temperatures $T^{(1)}_k$ are determined.

Items 2 – 5 are repeated with new functions and parameters, and iterations continue till the difference in functional J values becomes less than the specified error.

As a result, we get all optimal functions and optimal parameters corresponding to the minimum of functional J_{min}.

Application of optimal control methods for investigation of module characteristics

Usually in the Institute of Thermoelectricity (Ukraine) we design and investigate modules made of Bi_2Te_3–based materials. TE performances of such materials for cooling and generation are shown in Fig. 6.

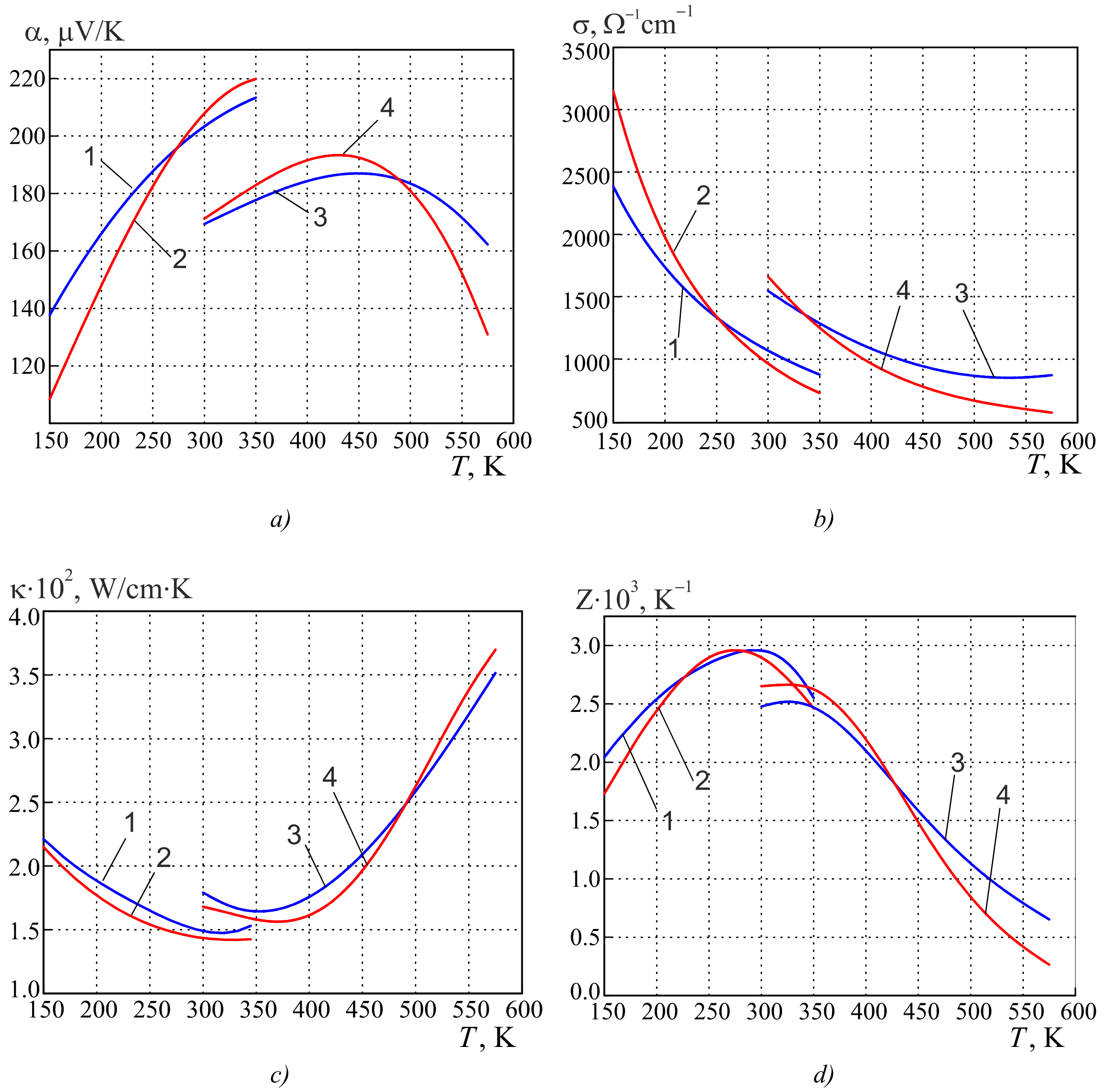


Fig. 6. Performances of Bi_2Te_3-based materials for cooling and generating modules. Materials for cooling modules: 1 – n-type $Bi_2Te_{2.7}Se_{0.3}$, 2 – p-type $Bi_{0.5}Sb_{1.5}Te_3$ and alloys used for generating converters: 3 – n-type $(Bi_2Te_3)_{0.90}(Sb_2Te_3)_{0.05}(Sb_2Se_3)_{0.05}$, 4 – p-type $(Bi_2Te_3)_{0.25}(Sb_2Te_3)_{0.72}(Sb_2Se_3)_{0.03}$.

Our latest research has focused on module miniaturization [5]. The miniaturization of thermoelectric converters is one of the modern trends to diminish the use of expensive TE material components, especially tellurium, reduce the cost of modules and expand the range of their applications. The main disadvantage of miniature thermoelectric converters operating in cooling or generating modes is their low energy efficiency, which is due to the effect of electrical and thermal resistances of contacts, interconnectors and insulating plates.

The effect of undesirable electrical and thermal resistances on the maximum efficiency of cooling and generating converters made of Bi_2Te_3-based materials was analyzed. The dependences of the maximum COP ε_{max} on a thermoelement length, calculated for temperature differences across the modules of 50 K, are shown in Fig. 7.

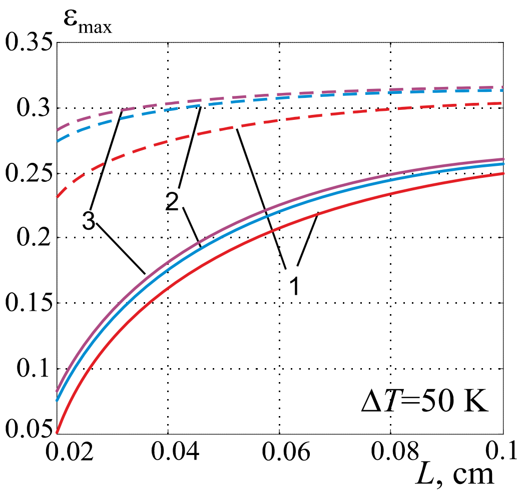


Fig. 7. Dependences of maximum COP ε_{max} on a leg length L. Contact resistance: r_c = 5×10^{-6} Ω cm^2 (solid lines), r_c = 10^{-7} Ω cm^2 (dashed lines). Insulating plates: 1 – Al_2O_3, 2 – AlN, 3 – pressed diamond powder. Temperature difference: ΔT=50 K. T_h=300.

A calculation was made for two values of resistivity r_c, namely, for the value r_c = 5×10^{-6} Ω cm^2 which is considered as typical for commercial TE modules and for the minimum value r_c = 10^{-7} Ω cm^2 which is caused by a potential barrier at the boundary between the TEM and the nickel anti-diffusion layer.

The influence of unwanted electrical and thermal resistances on the efficiency and power density was studied for generating converters. The dependences of maximum efficiency η_{max} and power density *w* on the leg length are shown in Fig. 8. Reducing the length of the thermoelements leads to a decrease in efficiency, which is especially sharp if the length is less than 0.1 cm and the contact resistance is high. It is obvious that with a decrease in the leg length, the density of the generated power increases. This testifies to the absolute advantage of converters with miniature thermoelements. But unwanted electrical and thermal resistances significantly affect this advantage, reducing the power density.

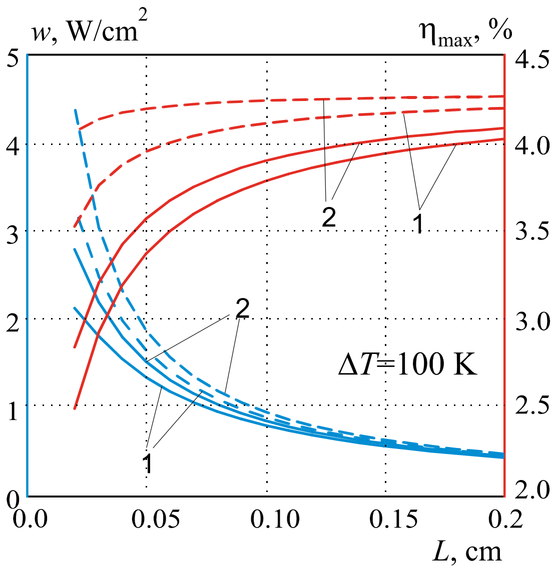


Fig. 8. Dependences of maximum efficiency η_{max} and power density w on the leg length L. Contact resistance: r_c = 5×10^{-6} Ω cm^2 (solid lines), r_c = 10^{-7} Ω cm^2 (dashed lines). Insulating plates: 1 – Al_2O_3, 2 – AlN. Temperature difference: ΔT=100 K . T_c=300 K.

We compared two methods for designing the modules – the classical Ioffe method and the method using optimal control. As an example we calculated the COP for the Ioffe ideal model of module (without undesirable electrical and thermal resistances) and for the real model. The results are presented in Table 1 as a ratio of COP ideal to COP real for different electrical and thermal resistances of contacts and insulating plates. It can be seen that the COP ε_{max} approaches the value ε_0 of an ideal model, only if the electrical contact resistance is minimal and the insulating plates are made of materials with high thermal conductivity. Otherwise, ε_{max} of the miniature module with a leg length of less than 0.05 cm is 2–6 times less than the value of ε_0. This fact testifies that using of optimal control method is quite reasonable.

Table 1

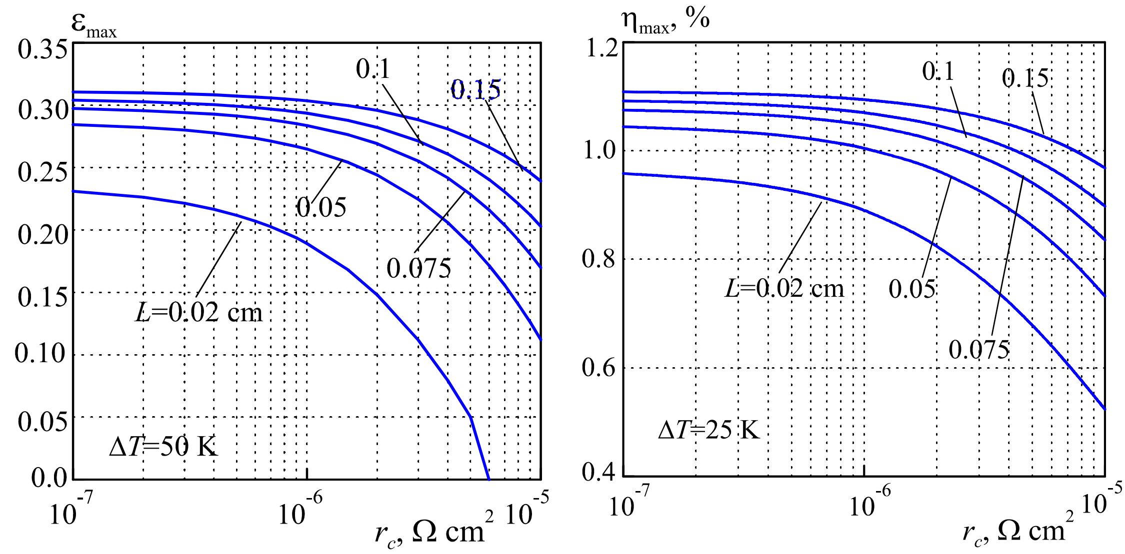
Ratio $\varepsilon_0/\varepsilon_{max}$ of ideal module COP ε_0 to real module COP ε_{max} in dependence of thermoelement length

Leg length L, cm	$\varepsilon_0/\varepsilon_{max}$ $r_c = 10^{-7}\ \Omega\ \mathrm{cm}^2$, AlN insulating plates	$\varepsilon_0/\varepsilon_{max}$ $r_c = 10^{-7}\ \Omega\ \mathrm{cm}^2$, Al_2O_3 insulating plates	$\varepsilon_0/\varepsilon_{max}$ $r_c = 5\times10^{-6}\ \Omega\ \mathrm{cm}^2$, AlN insulating plates	$\varepsilon_0/\varepsilon_{max}$ $r_c = 5\times10^{-6}\ \Omega\ \mathrm{cm}^2$, Al_2O_3 insulating plates
Temperature difference across a module ΔT=10 K, ε_0=4.149				
0.1	1.02	1.06	1.10	1.14
0.05	1.04	1.12	1.21	1.29
0.02	1.11	1.30	1.54	1.77
Temperature difference across a module ΔT=30 K, ε_0=0.961				
0.1	1.02	1.05	1.14	1.17
0.05	1.04	1.10	1.29	1.35
0.02	1.11	1.26	1.85	2.11
Temperature difference across a module ΔT=50 K, ε_0=0.324				
0.1	1.03	1.07	1.25	1.29
0.05	1.07	1.14	1.59	1.72
0.02	1.18	1.40	4.18	6.47
2-stage module ΔT=70 K, ε_0=0.153				
0.1	1.02	1.08	1.32	1.40
0.05	1.05	1.17	1.76	2.0
3-stage module ΔT=90 K, ε_0=0.0618				
0.1	1.03	1.09	1.47	1.57
0.05	1.05	1.19	2.22	2.54
4-stage module ΔT=105 K, ε_0=0.0284				
0.1	1.03	1.1	1.66	1.78
0.05	1.06	1.21	2.84	3.3

The analysis of these data also shows that the efficiency of miniature modules can be significantly improved if the unwanted resistances are reduced to their rational values. The decrease in electrical contact resistance is the predominant factor.

The dependences of COP and efficiency on contact resistivity for convertors with various thermoelement length are shown in Fig. 9. The data show that there is a rational value $r_{c\ opt}$ of the contact resistivity, such that for $r_c < r_{c\ opt}$ the increase in the efficiency becomes insignificant, namely, does not exceed 5%. The results of computer calculations have shown that the rational value of $r_{c\ opt}$ depends only on the length of the converter legs and does not depend either on the temperature drop in the converter or on the thermal resistance of the insulating plates.

The data in Fig. 9 were used to determine the rational values to which it is advisable to decrease the electrical contact resistivity for cooling and generator converters with different leg length. The results are presented in Table 2.



a) *b)*

Fig. 9. Dependences of COP (a) and efficiency (b) on contact resistance for convertors with various thermoelement length. Insulating plates are made of Al_2O_3

<u>*Table 2*</u>

Rational values of contact resistance $r_{c\ opt}$

Cooling module					
Thermoelement length L, cm	0.15	0.1	0.075	0.05	0.02
Rational contact resistivity $r_{c\ opt}$, $\Omega\cdot cm^2$	$2\cdot10^{-6}$	10^{-6}	$9\cdot10^{-7}$	$7\cdot10^{-7}$	$3\cdot10^{-7}$
Generating module					
Thermoelement length L, cm	0.15	0.1	0.075	0.05	0.02
Rational contact resistivity $r_{c\ opt}$, $\Omega\cdot cm^2$	$3\cdot10^{-6}$	$2\cdot10^{-6}$	$1.5\cdot10^{-6}$	10^{-6}	$6\cdot10^{-7}$

It is necessary to focus on such rational contact resistance values in the development of miniscale modules' technology.

Conclusions

1. This lecture outlines the main concepts of optimal control theory and explains how they are used to design thermoelectric converters for coolers and generators and calculate their characteristics. It is shown that the numerical method developed on the basis of optimal control theory for module design has a number of advantages compared to the use for this purpose of the A. Ioffe classical optimal relations. This method is suitable for the optimization of single- and multi-stage converters made of homogeneous or inhomogeneous materials. It takes into account the temperature dependence of material thermoelectric parameters and the additional thermoelectric effects in the material volume, as well as electrical and thermal losses in contacts, interconnectors, insulating plates and heat sinks on the hot and cold sides of the module.
2. The lecture gives examples of calculation the convertor characteristics and analyzes the influence of undesirable electrical and thermal resistances of contacts, interconnectors and insulating plates on the maximum COP and efficiency of converters made of Bi_2Te_3-based materials. It is concluded that the module energy efficiency is significantly improved if these resistances are reduced to their rational values. In particular, the COP of modules with miniature thermoelements increases by 2 – 6 times, and the efficiency of generator converters increases by 1.5 – 2 times.
3. It is shown that the reduction of electrical contact resistance is the predominant factor for increasing the efficiency of converters made of miniature thermocouples. The rational values have been determined, to which it is advisable to reduce the contact resistance. These contact resistance values should be adhered to when developing the technology of miniscale modules.

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МОДЕЛЮВАННЯ ХАРАКТЕРИСТИК ТЕРМОЕЛЕКТРИЧНОГО ПЕРЕТВОРЮВАЧА

(Лекція на Літній Термоелектричній школі,
30 червня, 2024, Краків, Польща)

За приблизними підрахунками річне світове виробництво термоелектричних перетворювачів (модулів) для потреб термоелектричної генерації та охолодження досягає понад 50 мільйонів штук. Термоелектричні перетворювачі механічно стійкі, високонадійні з терміном служби до 20 років. Головним недоліком є їх низька енергоефективність. Особливо це стосується мініатюрних модулів з довжиною термоелементів від 500 мкм до 200 мкм. Їх низька енергоефективність обумовлена дією електричних і теплових опорів контактів, комутацій та ізоляційних пластин. Одним із шляхів підвищення ефективності термоелектричних генераторів і охолоджувачів є оптимізація матеріалів та конструкції термоелектричних модулів для необхідних умов експлуатації. Для цього доцільно використовувати методи теорії оптимального керування. Вони придатні для оптимізації одно- і багатокаскадних перетворювачів, виготовлених з однорідних або неоднорідних, так званих функціонально градієнтних термоелектричних матеріалів (ФГТМ). Методи оптимального керування дозволяють враховувати температурні залежності термоелектричних параметрів матеріалів, додаткові об'ємні термоелектричні ефекти, яків виникають в ФГТМ, та вплив небажаних електричних і теплових опорів у модулях. У цій лекції висвітлюються основні поняття теорії оптимального керування та пояснюється, як вони використовуються для проєктування оптимальної конструкції модулів та моделювання їх характеристик. Розглянуто приклади розрахунку характеристик перетворювачів та проаналізовано вплив небажаних електричних і теплових опорів на максимальну енергетичну ефективність охолоджуючих і генераторних перетворювачів з матеріалів на основі Bi_2Te_3. *Показано, що ефективність модулів, особливо мініатюрних, можна значно підвищити, якщо ці небажані опори зменшити до раціональних значень. Переважаючим фактором є зниження електричного контактного опору. Визначено раціональні значення, до яких доцільно зменшити цей опір. Саме на такі раціональні значення контактного опору необхідно орієнтуватися в розробці технології модулів. Бібл. 9, рис. 9, табл. 2*

Ключові слова: термоелектричний перетворювач, енергоефективність термоелектричного модуля, методи теорії оптимального керування, холодильний коефіцієнт, електричний контактний опір, термічний опір комутаційних та ізоляційних пластин.

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