COMPUTER DESIGN OF SEGMENTED *PbTe* BASED THERMOELECTRIC MODULES

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• *Results of design of segmented thermoelectric modules and modules of functionally graded materials based on PbTe for the industrial, vehicular and other waste heat recovery are presented. Computer methods based on optimal control theory are used to determine the optimal parameters of thermoelectric materials for segments and the optimal inhomogeneity functions of functionally graded materials whereby maximum module efficiency is achieved.*

Introduction

At the present time, studies aimed at seeking the ways for improving the efficiency of thermal into electrical energy conversion become increasingly relevant. There is a good outlook for using industrial, vehicular and other kinds of waste heat recovery for their recuperation, in particular, conversion into electric energy with the aid of thermoelectricity [1 – 6]. The temperature level of such heat sources is 500 to 600°C.

Among thermoelectric materials used for creation of generator modules for such hot temperature level, traditional is *PbTe* based material. It is mostly employed in thermal generators of space application, for power supply to cathode protection systems, etc. However, wide practical use of such generators is restrained by the insufficient efficiency which for terrestrial thermal generators based on *PbTe* with different heat sources, including catalytic ones, does not exceed 3.5% [7].

The purpose of this work is to design *PbTe* thermoelectric modules and estimate the possibility of their efficiency improvement through use and optimization of segmented thermoelements.

Research results

Computer design of generator modules made of *PbTe* based materials was done with the use of optimal control theory methods [8]. In this way concentration segmented thermoelements were designed and for each segment optimal impurity concentrations were determined that agree with their optimal geometric dimensions.

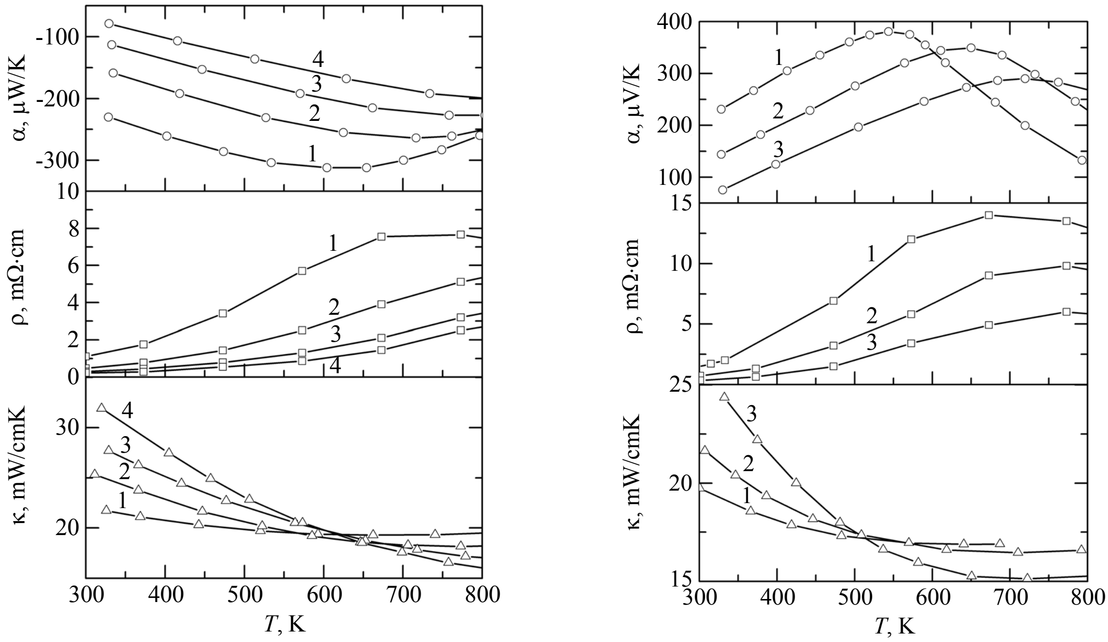
The design employed the experimentally measured concentration-temperature dependences of α, σ, κ parameters of *n*-type *PbTe* samples doped with iodine [9] and sulphur [10]; as well as of *p*-type *PbTe* samples doped with sodium [9] and selenium [11]. In Figs. 1, 2 these dependences are given for materials with different doping degrees, hence different current carrier concentrations.

The represented temperature dependences (Fig.1, 2) were approximated by two-dimensional polynomials in the form of $\alpha^{n,p} = \alpha^{n,p}(\sigma_0^{n,p}, T)$, $\sigma^{n,p} = \sigma^{n,p}(\sigma_0^{n,p}, T)$, $\kappa^{n,p} = \kappa^{n,p}(\sigma_0^{n,p}, T)$ and polynomial coefficients were introduced into computer program as the input data. The designation of module legs for the above materials is given in Table 1.

<u>*Table 1*</u>

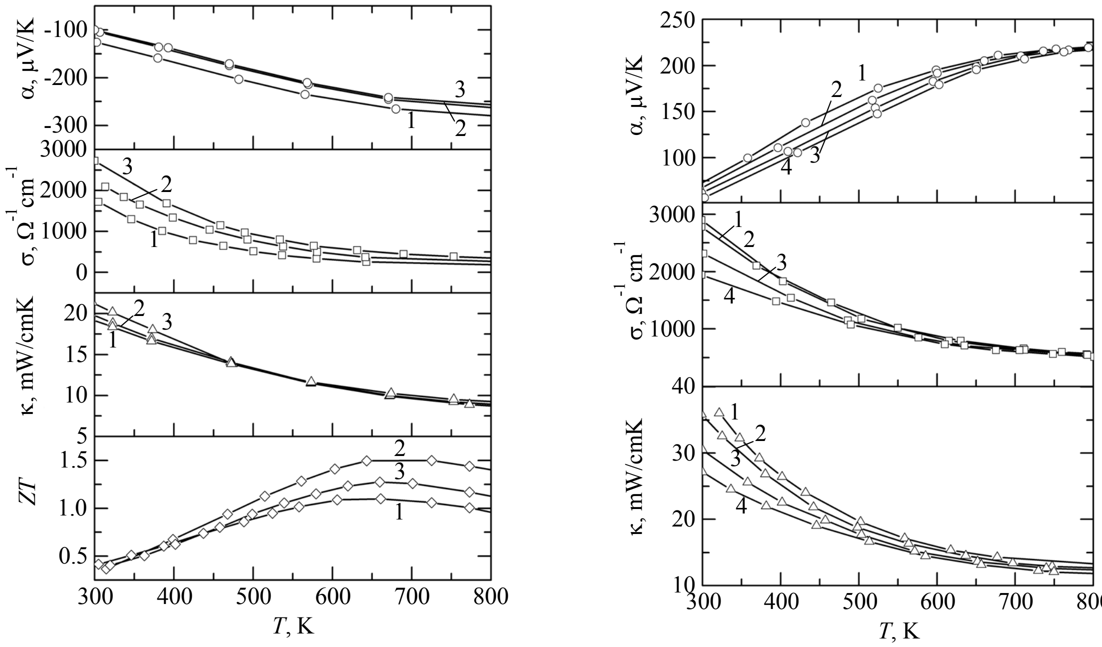
Legs designation of generator modules made of PbTe based materials.

Designation	*n*-type leg	Designation	*p*-type leg
S1	*PbTe* <*x* mol.% PbI_2> (x = 0.01 – 0.1) [9]	S2	*PbTe* <*x* at.% *Na*> (x = 0.1 – 1) [9]
S3	*PbTe* <*x* mol.% *PbS* + 0.055 mol.% PbI_2> (x = 4 – 16) [10]	S4	*PbTe* <*x* at.% *PbSe* + 2 at.% *Na*> (x = 0 – 25) [11]



a) *b)*

Fig. 1. Temperature dependences of thermoelectric parameters of samples:
a) PbTe <x mol.% PbI_2> (1 – x = 0.01; 2 – x = 0.03; 3 – x = 0.055; 4 – x = 0.1) [9];
b) PbTe<x at.% Na> (1 – x = 0.1; 2 – x = 0.3; 3 – x = 1) [9].



a) *b)*

Fig. 2. Temperature dependences of thermoelectric parameters of samples:
a) PbTe <x mol.%PbS + 0.055 mol.%PbI_2> (1 – x = 4; 2 – x = 8; 3 – x = 16) [10];
b) PbTe <x at.%PbSe + 2at.%Na> (1 – x = 0; 2 – x = 5; 3 – x = 15; 4 – x = 25) [11].

Optimal parameter values of materials for single- and double-segmented legs of generator thermoelements for the working temperature range 323 to 773 K, the optimal heights of segments for double-segmented thermoelements are given in Table 2. The values of contact resistances in the calculations were assumed equal to $5\cdot10^{-6}$ Ω·cm on thermoelement junctions and $1\cdot10^{-5}$ Ω·cm – on the boundaries between leg segments.

Table 2

Parameter values of materials based on PbTe at T = 300 K for generator modules

Leg and segment designation, dopant concentration			Optimal parameter values				Segment height, mm
			σ_0, $\Omega^{-1}\cdot cm^{-1}$	α, $\mu V/K$	κ, mW/cm·K	Z, $10^{-3}K^{-1}$	
n-type leg							
S1-S2	1 segment	$x = 0.0872$	4430	68.9	30.9	0.68	5.6
S1-S4	1 segment	$x = 0.0878$	4448	69	30.9	0.685	5.6
S3-S2	1 segment	$x = 7.17$	1982	106	19.6	1.137	5.6
	1 segment*	$x = 14.05$*	2300*	82.5*	18.5*	0.85*	5.6*
S3-S4	1 segment	$x = 7.13$	1972	107	19.83	1.138	5.6
	1 segment*	$x = 14.06$*	2300*	82.4*	18.4*	0.85*	5.6*
S1-S2	2 segments: hot and cold	$x = 0.0813$ $x = 0.0143$	4260 1090	68.7 182	30.5 23.6	0.659 1.29	2.5 3.1
S1-S4	2 segments: hot and cold	$x = 0.0768$ $x = 0.0127$	4130 1020	68.5 188	30.2 23.4	0.643 1.54	2.5 3.1
S3-S2	2 segments: hot and cold	$x = 10.799$ $x = 6.287$	2150 1940	94 110	19.1 20	0.994 1.172	2.4 3.2
S3-S4	2 segments: hot and cold	$x = 10.62$ $x = 5.5$	2150 1860	94.3 115	19.2 20.3	0.998 1.208	2.78 2.82
p-type leg							
S1-S2	1 segment	$x = 0.6857$	1958	89.2	24.2	0.644	5.6
S1-S4	1 segment	$x = 6.516$	2810	65.2	35.1	0.34	5.6
S3-S2	1 segment	$x = 0.6872$	1960	89	24.2	0.642	5.6
	1 segment*	$x = 0.6805$*	1950*	89.7*	84.2*	0.648*	5.6*
S3-S4	1 segment	$x = 6.53$	2810	65.2	35.1	0.34	5.6
	1 segment*	$x = 6.43$*	2815*	65.3*	35.15*	0.341*	5.6*
S1-S2	2 segments: hot and cold	$x = 0.7966$ $x = 0.3213$	2220 1410	78.9 123	24.8 22.1	0.557 0.965	2.4 3.2
S1-S4	2 segments: hot and cold	$x = 7.664$ $x = 1.686$	2740 2700	64.7 68.7	34.4 38	0.333 0.335	3 2.6
S3-S2	2 segments: hot and cold	$x = 0.7987$ $x = 0.3457$	2225 1440	78.7 121	24.85 22.3	0.555 0.945	2.3 3.3
S3-S4	2 segments: hot and cold	$x = 7.1$ $x = 0.7$	2775 2730	65 69.4	34.7 38.6	0.338 0.341	2.92 2.68

* – other dopant concentration

From the above data it is seen that in the high-temperature segments one should use materials with a higher electric conductivity and, accordingly, a lower absolute value of the Seebeck coefficient. On closing of electric circuit, current will flow in the direction of the Seebeck coefficient increase. Partial thermoEMFs caused by the difference in α on the boundaries between leg segments will be summed up, increasing thermoelement efficiency.

For comparison, thermoelectric modules were designed for heat recuperators of functionally graded materials (FGM) based on *PbTe.* If *PbTe*<PbI_2> material is selected for *n*-type leg, and *PbTe*<*Na*> (*S*1-*S*2) for *p*-type leg, the optimal distributions of carrier concentration in *n*-type legs are created by the distribution of PbI_2 dopants within 0.01 – 0.1 mol.%, and in *p*-type legs – by the distribution of *Na* dopants within 0.1 – 1 at.% (Fig. 3) by the law:

$$C_n = \frac{0.91 + 5.07\bar{x}^2}{1 - 1.24\bar{x}^2 + 0.86\bar{x}^4},$$
$$C_p = 1.01 - 13\bar{x}^2 + 420\bar{x}^4 - 1637\bar{x}^6 + 2902\bar{x}^8 - 2695\bar{x}^{10} + 1271\bar{x}^{12} - 240\bar{x}^{14}, \quad (1)$$

where $\bar{x} = x / L$ is dimensionless coordinate along the leg height *L*.

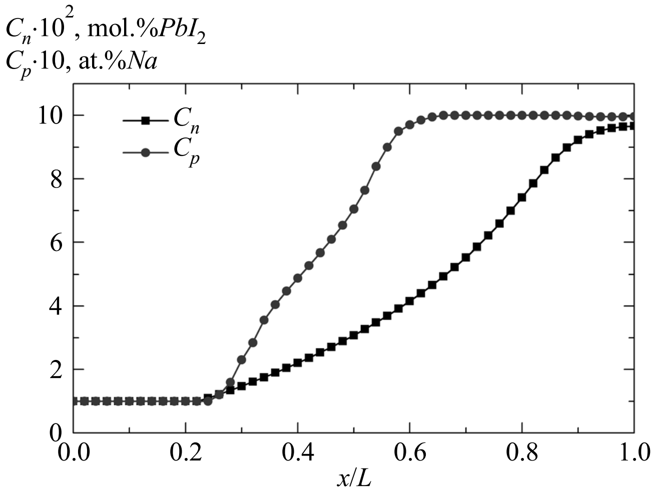


Fig. 3. Distribution of impurity percentage (PbTe <x mol.% PbI_2> and PbTe <x at.% Na>) in FGM legs for generator modules.

Determined in maximum efficiency mode, optimal energy characteristics (current, voltage, power, efficiency) of single- and double-segmented modules, as well as FGM modules with the number of thermoelements N_{TE} = 32 couples and the height of legs 5.6 mm, are listed in Table 3. In so doing, the values of generated current *I,* voltage *U* and power *W* that are optimal for maximum efficiency mode and can be expected on the external load, were determined on the basis of relations (2)

$$S_{n,p} = \frac{I \cdot l_k^{n,p}}{\sum_{k=1}^{N_{n,p}} j_k^{n,p}}, \qquad I = \frac{S_{n,p}}{l_k^{n,p}} j_k^{n,p},$$
$$n_k = \frac{U}{q(l) - q(0)}, \qquad U = n_k \cdot \left[q(l) - q(0) \right], \quad (2)$$

where $S_{n,p}$ are cross-section areas of legs; $l_k^{n,p}$ are the heights of individual segments; n_k is the number of thermoelements in a module; *q*(*l*), *q*(0) are specific (related to current strength) heat fluxes on thermoelement junctions; $j_k^{n,p}$ are optimal current densities.

From the analysis of Table 3 it follows that in going from single- to double-segmented modules, the efficiency is increased by a factor of 1.6 (with identical module height). Preferable for a single-segmented module is S3-S2 variant, and with increase in the number of segments, preference should be given to S1-S2. The *PbTe*<*x* mol.%*PbS* + 0.055 mol.%PbI_2> material (S3) is characterized by a considerable effect of concentration on module parameters, namely when it is used in single-segmented modules with concentration $x \approx 14.05$ (*), module parameters are much worse than at $x \approx 7.15$; in the design of double-segmented modules on its basis (S3-S2), compatibility between segment materials is selected such that the cold segments are matched by concentrations $x \approx 6.3$, and the hot segments – by $x \approx 10.8$. Hence, S3 material can be efficiently used in single-segmented modules; with increase in the number of segments, the relative efficiency growth of modules on its basis is reduced.

Among the double-segmented modules, the best thermoelectric properties are exhibited by generator modules, where iodine-doped lead telluride is selected as *n*-leg, and sodium-doped lead telluride (S1-S2) is selected as *p*-leg. The results of investigation of the effect of leg height on the generated power and efficiency are given in Fig. 4.

Table 3

Characteristics of generator modules made of optimal PbTe based materials for the working temperature range 323 to 773 K

Module type		Generated electric power W, W	Current I, A	Voltage U, V	Efficiency η, %
Modules with single-segmented legs	S1-S2	20.31	6.77	3	8.766
	S1-S4	18	7.27	2.47	8.211
	S3-S2	14.64	4.22	3.47	8.908
		13.5*	3.94*	3.42*	8.325*
	S3-S4	14.4	4.88	2.95	8.452
		13.2*	4.56*	2.89*	7.816*
Modules with double-segmented legs	S1-S2	37.76	8.7	4.34	14.355
	S1-S4	32.8	10	3.28	13.58
	S3-S2	26.8	6.44	4.16	13.414
	S3-S4	24.3	7.79	3.12	12.473
Modules with FGM	S1-S2	38.1	9.41	4.05	15.83

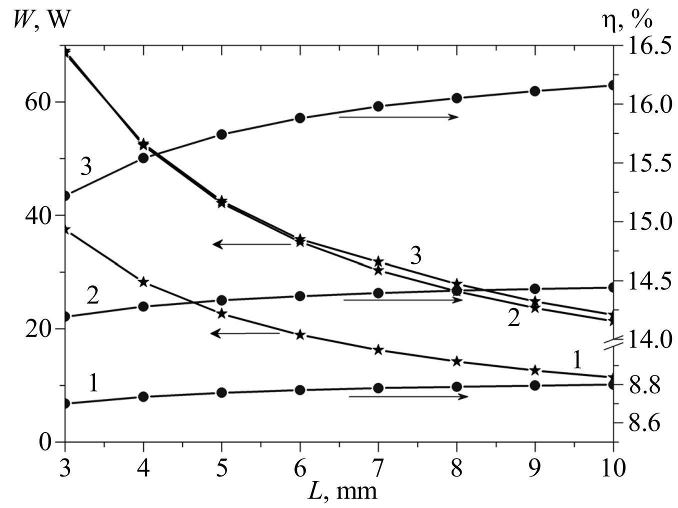


Fig. 4. Height dependence of generated power and efficiency of generator modules (S1-S2): 1 – single-segmented; 2 – double-segmented; 3 – FGM-based.

From Fig. 4 it is seen that the efficiency is weakly dependent on the height of legs (for single- and double-segmented modules the difference in the values does not exceed 2%, in the case of FGM – 6%), and higher power is achieved at lower heights. Comparison of double-segmented modules and FGM modules shows that the character of their dependences $W = f(L)$ is the same with different efficiency values ($\eta_{FGM} = (1.07 – 1.12)\cdot\eta_{2sec}$).

Conclusions

Computer design method was used to determine the optimal parameters of materials for single- and double-segmented thermoelectric generator modules based on *PbTe.* For a single-segmented module it is optimal to use *n-PbTe* doped with sulphur and *p-PbTe* doped with *Na*; for a double-segmented – with I_2 and *Na,* respectively. As compared to single-segmented modules, using two segments in *PbTe* based modules at the hot side temperature 500°C and cold side temperature 50°C allows improving their efficiency by a factor of 1.6.

Maximum efficiency of modules made of functionally-graded materials based on *PbTe* is 15.8%, which is a factor of 1.1 greater as compared to double-segmented modules.

The use of segmented modules made of optimally inhomogeneous *PbTe* based materials is a promising way of increasing the efficiency of thermoelectric generators for heat waste recovery whose temperature level is 500 to 600°C.

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