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ON THE SIMULATION OF PERMEABLE THERMOELEMENTS

The results of theoretical research on permeable thermoelements are presented. In Comsol Multiphysics application software package a 3D model of thermoelement is created with regard to temperature dependences of material parameters, the availability of connecting buses, heat spreaders and contact resistances. A method of mathematical optimal control theory and computer design for solving multi-factor optimization problems in a 1D model is described. Computer programs are created to determine design and thermophysical parameters affording maximal values to thermodynamic characteristics of energy conversion. Computer calculations of optimal parameters of permeable thermoelements for various materials based on Bi – Te – Se – Sb are performed. Calculated data point to possible improvement of thermoelectric energy conversion efficiency by a factor of 1.2 – 1.5 as compared to conventional thermoelements.

Key words: permeable thermoelement, energy characteristics, optimization, design.

Introduction

A promising direction for efficiency increase of thermoelectric energy conversion is the use of physical models of thermoelements wherein heat exchange with the heat source and heat sink occurs not only through the junctions of legs, as in conventional thermoelements, but also in the bulk of the legs material [1, 2]. The variants of such models include permeable thermoelements having channels for pumping liquid or gas heat carrier [3]. The availability of heat exchange in the bulk of the leg increases the intensity of heat transfer, leads to redistribution of temperature fields, potentials and thermal flows, thus affecting the energy characteristics of thermoelement. Having control over thermophysical parameters (heat carrier pumping speed, heat exchange intensity, electric current density, etc.) one can create such operating conditions whereby energy conversion efficiency will be improved.

The first theoretical investigations of permeable thermoelements for gas flows [4 – 6] showed the promising outlook for their creation, since they predict coefficient of performance improvement by 30 – 40 % [7] on air cooling and generator efficiency increase by 20 – 30 % [8] when using low-grade thermal energy of gases. However, such investigations were performed for the simplest model of permeable thermoelement in a one-dimensional approximation without regard to temperature dependences of material parameters, connecting heat spreaders, etc.

Therefore, for a more correct solution of such problems in [9] we pioneered the use of mathematical optimal control theory and studied permeable thermoelements in a 1-D model of semiconductors with regard to their temperature dependences for the homogeneous and functionally graded materials (FGM). This made it possible to create theory of permeable thermoelements of FGM and show the possibilities of energy characteristics improvement in electric energy generation and heat carrier cooling modes by a factor of 1.2 – 1.5.

Creation of a 3-D model of permeable thermoelement is complicated by the necessity to solve a conjugate problem of heat, electro- and mass exchange in solid-heat carrier system. This problem was solved in Comsol Multiphysics application software package for permeable plane thermoelement [10]. However, parameter optimization to find maximum values of energy characteristics in such 3-D cases is difficult. The present paper describes peculiarities of methods for solving problems in 3-D and 1-D cases for different models of permeable thermoelements.

Physical model, mathematical description and the results of problem solution

For the inhomogeneous isotropic permeable thermoelectric medium (Fig. 1) where there is a steady-state flow of heat, charged particles and energy caused by the presence of temperature gradients ∇T and electrochemical potential $\nabla\zeta$, exchange and energy conversion processes are described by the fundamental laws of energy and electric charge conversion.

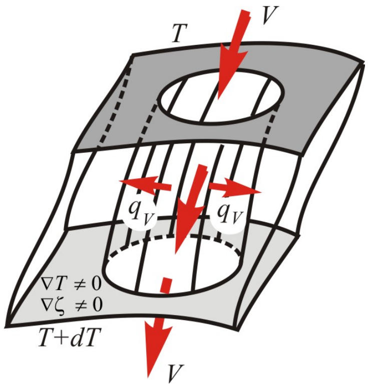


Fig. 1. Permeable thermoelectric medium.

In the steady-state case the distribution of temperature T in thermoelectric material is determined by a system of differential equations in partial derivatives

$$\left.\begin{aligned} &\nabla(\kappa\nabla T) + \frac{\vec{\boldsymbol{i}}^{\,2}}{\sigma} - T\frac{\partial\alpha}{\partial T}(\vec{\boldsymbol{i}}\nabla T) - T(\vec{\boldsymbol{i}}\nabla\big|_{T=const}\,\alpha) = 0, \\ &\nabla(-\sigma\nabla\zeta - \sigma\alpha\nabla T) = 0, \end{aligned}\right\} \qquad 1)$$

where $\vec{\boldsymbol{q}} = -\kappa\nabla T + \alpha T\vec{\boldsymbol{i}}$ is heat flux density vector; $\vec{\boldsymbol{i}} = -\sigma\nabla\zeta - \sigma\alpha T$ is current density vector; α is the Seebeck coefficient, σ is electric conductivity coefficient; κ is thermal conductivity coefficient .

The presence of heat exchange between thermoelectric material and heat carrier necessitates solving (1) conjugate to equations of continuity, motion and thermal conductivity for heat that can be written as follows:

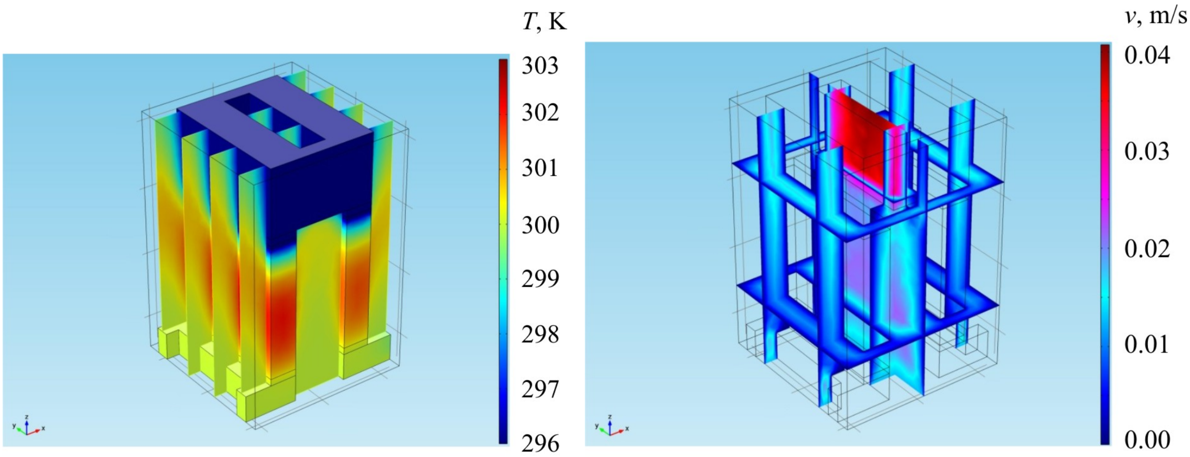
$$\left.\begin{aligned} &\mathrm{div}(\rho_t\vec{\boldsymbol{V}}) = 0, \\ &\rho_t\vec{\boldsymbol{F}} - \nabla p + \mu\nabla^2\vec{\boldsymbol{V}} + \frac{1}{3}\mu\vec{\nabla}(\mathrm{div}(\vec{\boldsymbol{V}})) = 0, \\ &\rho_t\vec{\boldsymbol{F}}\vec{\boldsymbol{V}} + \mathrm{div}(\Lambda\vec{\boldsymbol{V}}) + \mathrm{div}(\kappa_t\nabla t) + \rho_t q_V = 0, \end{aligned}\right\} \qquad (2)$$

where ρ_t is heat carrier density; $\vec{\boldsymbol{V}}$ is heat carrier velocity; $\vec{\boldsymbol{F}}$ is mass force; ρ is pressure; Λ is stress tensor; κ_t is heat carrier thermal conductivity; q_V are internal heat sources; U is internal energy.

To solve such a problem, it is reasonable to use specially developed application software programs of the type Femlab, ANSYS, COMSOL Multiphysics.

A 3-D simulation of generator thermoelement with a lateral heat exchange was performed in [10] on the basis of COMSOL Multiphysics program.

The obtained distribution of temperatures in the leg material based on $Bi-Te$ and in heat carrier (Fig. 2*a*), the distribution of heat carrier velocity (Fig. 2*b*) and potential distribution allow determination of thermodynamic conversion characteristics.



a) *b)*

Fig. 2. Temperature distribution in thermoelement and heat carrier (a), velocity field distribution in heat carrier (b).

The calculated results point to the fact that with the use of lateral heat exchange large efficiency values are attained when heat exchange takes place at 0.5 of the leg height, and the other part is thermally insulated. The data is also obtained for other thermoelement designs and heat carrier temperature which varies in the range of 700 – 1100 K. The data suggests that the use of lateral heat exchange can yield efficiency increase by 20 – 30 % and electric power increase by 40 – 50 %.

The calculated results indicate a need to solve a multi-parameter optimization problem on finding optimal conditions for thermoelement operation and maximum values of its energy characteristics. However, to perform such multi-parameter optimization for a 3-D model is extremely difficult. The use of a 1-D model makes it possible to perform multi-parameter optimization of the energy characteristics of thermoelements, determine for them such operating conditions which enable one to attain maximum values of energy conversion efficiency.

In a 1-D case the energy characteristics of permeable thermoelement are determined on the basis of solving a system of differential equations for heat carrier and leg material of *n*- and *p*-types given below:

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

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

For solving optimization problem to find the optimal operating conditions of thermoelement, the works employ Pontryagin's maximum principle of mathematical optimal control theory which yields the necessary optimality conditions:

1) optimal values of specific current density in thermoelement legs j must meet the equalities

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

where J is functional characterizing the efficiency of energy conversion process (efficiency for generators, coefficient of performance for cooling, etc); $\left(f_1, f_2, f_3\right)_{n,p}$ are the right-hand sides of equations (1), $\psi=\left(\psi_1,\psi_2,\psi_3\right)_{n,p}$ is vector function of pulses [12] found from the solution of auxiliary system of differential equations

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

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) optimal values of required parameters $\omega_i=(\omega_1,\ldots,\omega_r)$, are found from the system of integral-differential equations

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

Based on the above ratios, with the use of successive approximations methods, numerical methods of solving the systems of differential equations (3) and (5), the Newton method of solving the systems of integral differential equations (6), computer program for design of permeable thermoelement has been developed [10].

The results of such calculations of permeable generator thermoelement of $Bi-Te-Se-Sb$ based materials under optimal operating conditions are given in Fig. 3.

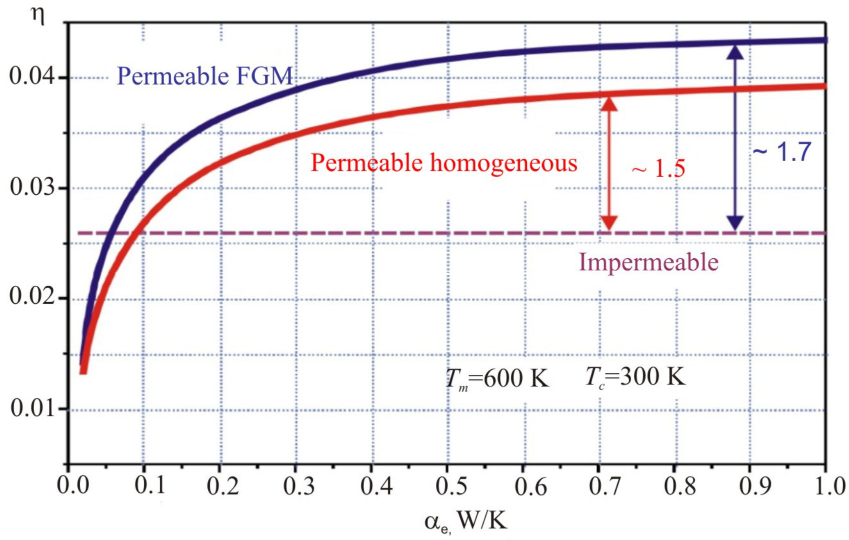


Fig. 3. Thermoelements efficiency versus the effective heat exchange coefficient.

As is evident, the efficiency of energy conversion with the use of permeable thermoelements made of homogeneous and functionally-graded materials can be increased by a factor of 1.2 – 1.5 as compared to impermeable thermoelements.

Conclusions

A physical model and method for calculation and design of permeable thermoelement where heat carrier is pumped through the legs of semiconductor material is described. A comparison between the results of calculation of a 3-D model and a one-dimensional thermoelement model (1-D) shows that a 1-D model with regard to the bulk thermoelectric effects realistically describes the processes of thermal and electric conductivity in thermoelectric medium.

For $Bi - Te - Se - Sb$ based materials the effect of design parameters (channel diameter and their number, leg height and the number of segments) on the energy characteristics under optimal operating conditions in terms of thermoelement efficiency is calculated. The rational values of these parameters are determined which make it possible to establish the necessary material science requirements for creation of thermoelement.

Comparison to conventional thermoelements in terms of thermodynamic efficiency of energy conversion has shown the possibility of efficiency increase by a factor of 1.2 – 1.5.

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