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Model for Calculating Thermoelectric Properties of Nanostructured Material

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For the barrier-well-barrier model of nanostructured thermoelectric material, based on Gaussian, Poschl-Teller potentials and rectangular barriers and well, thermoelectric characteristics were calculated. For quantum barrier-well-barrier structures based on Gaussian and PoschlTeller potentials, a program was developed to calculate thermoelectric characteristics using the Thomas algorithm for calculating the transmission coefficient of particles through the quantum structure and numerical integration of expressions for electrical conductivity and Seebeck coefficient, with corresponding graphical illustration of the results obtained. The calculations program is implemented on the Maple computer mathematics platform. For the quantum structure based on rectangular potentials, using the quantum impedance method, an expression was obtained for the transmission coefficient of particles through such a structure and applied for the calculation of electrical conductivity, Seebeck coefficient, and power factor using symbolic mathematics of the Maple package. The influence of resonant tunneling of particles through the proposed triple-barrier structure on its thermoelectric characteristics is taken into account. An analysis of the obtained calculation results is presented.

Keywords: quantum tunneling mechanism of thermoelectric phenomena, model of nanostructured material, Seebeck coefficient, power factor.

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Introduction

Since it became clear that if barriers are included in bulk material, the properties of electronic transport can be significantly altered, a number of studies have investigated the role of "energy filtering"of carriers [5] in thermoelectric phenomena. A theory of the quantum-tunneling mechanism of thermoelectric phenomena was developed for several quantum systems based on superlattices with quantum wells, quantum dots, and other thermotunneling objects [1] – [4]. Moreover, the emergence of a new technology based on grinding thermoelectric material to sizes of 10-20 nm followed by hot pressing (see, for example, [6]) ensures its nanoscale structuring. That is, the bulk material is formed by nanoscale grains with corresponding intergranular gaps. At these grain and intergranular gap sizes, the system can be considered as a quantum-mechanical system, which includes a quantum well surrounded by two barriers. In such systems, quantum transport of the tunneling type is realized. This model also accounts for the possibility of resonant transmission through the barrier-well-barrier quantum system.

I. Model of Nanostructured Thermoelectric Material

As already noted, the presence of barriers significantly alters the thermoelectric properties of the material. In the case of a nanostructured material, the nanograin itself will be described by quantum laws and may contain bound states, which will cause resonant processes when carriers pass through it. By defining the shape of the barriers and the well with different functions, several useful models of the nanostructured material can be obtained. For example, by defining the well shape with the Gaussian potential, one can obtain a model describing a quantum dot surrounded by two barriers. If both the barriers and the well are considered rectangular, then an

exactly solvable model of the nanostructured material can be obtained. Several advantages can be obtained for the model described by the Poschl-Teller potential, considering that under certain parameters such potential becomes reflectionless. A graphical representation of one of these models is shown in Figure 1, which depicts a quantum-mechanical model constructed using the function (4). Here, distances are given in relative units $x = \boldsymbol{x}/a_0$ where a_0=1nm, and V_0 is the potential parameter related to the height of the potential barrier, also defined in relative units $V_0 = U_0/E_0$, where $E_0 = \hbar^2/2ma_0$, and ς is the half-width of the Gaussian function defined in relative units $\varsigma = w/a_0$.

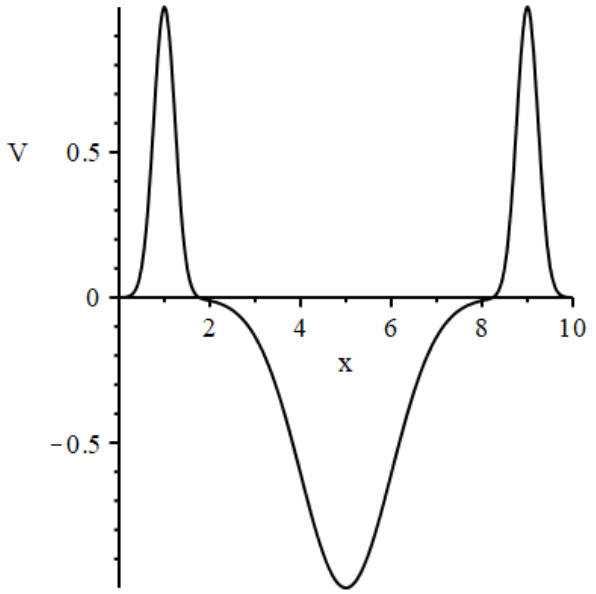

Fig. 1. The potential-energy diagram of a nanoparticle with intergranular barriers based on the Gaussian function: the height of the barriers and the depth of the wells are one relative unit each, the half-width of the barriers is $\varsigma = 1/3$, and the half-width of the wells is $\varsigma = 1$.

II. Fundamental Relations for Quantum Transport

Kinetic phenomena during the passage of carriers through a barrier-wellbarrier quantum system are described by the quantum-tunneling mechanism of transport phenomena. According to the ideas of Landauer's quantum transport theory [8], [9], the density of the tunneling current in the case when an external electric field and a temperature gradient are applied to the system is given by the expression

$$j = \frac{1}{4\pi^3}\int e v_x \tau(E_x)\left[f_0\left(\frac{E-\mu}{k_0T}\right) - f_0\left(\frac{E-(\mu+\Delta V)}{k_0T}\right)\right] d^3k \quad (1)$$

where $f_0\left(\frac{Ek0-T\mu}{k_0T}\right) = \frac{1}{e^{\frac{Ek0-T\mu}{k_0T}+1}}$ is the Fermi-Dirac distribution function, $\tau(E)$ is the transmission coefficient of the quantum structure, e is the elementary charge, υ_x is the velocity projection in the direction $0x$, μ is the chemical potential of the carriers, ΔV is the potential difference applied to the sample, T is the absolute temperature, and k_0 is the Boltzmann constant.

For typical values of potential differences applied to the sample and currents passing through it with nanoparticle sizes of $10-20\ nm$, the voltage drop on one grain will be from $10^{-6}\ V$ to $\sim 10^{-4}\ V$. At a temperature difference of $100K$ across the sample, the temperature difference for one nanograin will be about $10^{-3}K$, and $k_0T \sim 10^{-7}\ eV$. Therefore, considering the above, the inequalities $e\triangle V << k_0T$ and $k0\triangle T << k0T$ will hold true, and in the difference of distribution functions, it is sufficient to limit to linear terms in $\triangle V$ and $\triangle T$. Then we obtain

$$j = \frac{me}{2\pi^2\hbar^3}\int_0^{\infty} dE_x \tau(E_x)\int_0^{E_x}\frac{\partial f_0(E)}{\partial E}\left(e\Delta V + \frac{E-\mu}{T}\,\Delta T\right) dE$$

In this formula, E_x is the kinetic energy of the carrier's motion along the $0x$ axis, and $E = E_x + E_\perp$ where $E_\perp$ corresponds to the energy that accounts for the degrees of motion in the Y,Z plane. The equation for the heat flux density j_q in the same approximation will be as follows

$$j = \frac{4\pi me}{(2\pi\hbar)^3}\int_0^{\infty} dE_x\,\tau(E_x)\int_0^{E_x}(E-\mu)\frac{\partial f_0(E)}{\partial E}\left(e\Delta V + \frac{E-\mu}{T}\,\Delta T\right) dE.$$

The calculation formulas for electrical conductivity and the Seebeck coefficient take the following form

$$\sigma = \sigma_0\int_0^{E_x}\tau(E_x) f_0\left(\frac{E-\mu}{k_0T}\right) dE_x \quad (2)$$

where $\sigma_0 = \frac{me^4aE_0}{4\pi^2\,\hbar^3}$ and is approximately equal to $2000\ (Om\cdot m)^{-1}$.

$$S = S_0\frac{\int_0^{E_x}\tau(E_x)\left[\left(\frac{E_x-\mu}{k_0T}\right)f_0\left(\frac{E-\mu}{k_0T}\right)+ln\left(1+exp\left(-\frac{E_x-\mu}{k_0T}\right)\right)\right]dE_x}{\int_0^{E_x}\tau(E_x)f_0\left(\frac{E-\mu}{k_0T}\right)dE_x} \quad (3)$$

where $S = \frac{k_0}{e}$ and is approximately equal to 100 $\mu V/K$.

The expressions for σ and S include the transmission coefficient of the particle through the barrier structure $\tau(E)$. For complex potential profiles as in our proposed case, the expression for $\tau(E)$ can mostly be obtained only by numerical methods.

The calculation of the expressions for electrical conductivity and the Seebeck coefficient will be performed in relative units.

III. Modeling Nanostructured Thermoelectric Material

3.1. Model of Nanostructured Thermoelectric Material Based on Gaussian Potential.

When modeling a nanostructured material, the nanograin can be described using the Gaussian potential [7], which can result in bound states. Therefore, we will use this potential to define both the potential barrier and the quantum well. Hence, the potential of the nanostructure will be described by the function

$$\mathrm{V(x)} = V_0 \exp(-9(x-1)^2) - \exp(-(x-5)^2) + V_0 \exp(-9(x-9)^2) \quad (4)$$

which describes a Gaussian-type barrier with a half-width of one relative unit centered at the point $x/x_0 = 1$, a Gaussian-type quantum well with a width of six relative units centered at the point $x/x_0 = 5$, and a Gaussian-type barrier with a half-width of one relative unit centered at the point $x/x_0 = 9$. Here, $x_0 = 1nm$, and V_0 is the potential parameter related to the height of the potential barrier, also defined in relative units as U_0/E_0. For the numerical solution, the Schrodinger equation is reformulated in so-called finite differences.

$$\frac{\psi_{n-1}-2\psi_n+\psi_{n+1}}{\Delta^2} + \frac{2m}{\hbar^2}(E-V_n)\psi_n = 0, \ \ (n = 1, 2, \dots N-1) \quad (5)$$

where Δ is the discretization step, n is the node number of the grid, V_n is the value of the potential energy, and n is the value of the wave function at the grid nodes.

Or in dimensionless form

$$\psi_{n-1} - u_n\psi_n + \psi_{n+1} = 0, \quad (n = 1, 2, \dots N-1) \quad (6)$$

where $u_n = \varepsilon - v_n - 2$, $v_n = {V_n}/{E_0}$, $\varepsilon = {E}/{E_0}$.

The finite difference equations (6) were solved approximately using the Thomas algorithm [12].

If $V(x)$ is non-zero in the interval $[0, a]$ and if the incident flux is normalized to one, then in the interval $(-\infty; 0]$

$$\psi_1(x) = e^{ikx} + re^{-ikx}$$

and for $x > a$ $\psi_3(x) = te^{ik(x-a)}$.

From the conditions of continuity of the wave function and its derivative at the point $x = 0$, we arrive at the following boundary condition

$$\psi'(0) + ik\,(0) = 2ik. \quad (7)$$

Similarly, at the right edge of the interval

$$\psi'(a) - ik\,(a) = 0. \quad (8)$$

To implement the Thomas algorithm for the finite difference analog of the Schrodinger equation and obtain the boundary conditions of the boundary value problem, a "dummy"grid node x_{-1} is introduced, and the derivative at the left edge of the interval $\psi'(0)$ is approximated by a three-point expression

$$\psi'(0) = \frac{\psi_1-\psi_{-1}}{2\Delta^2}.$$

Using the expression for $\psi'(0)$, we arrive at the following boundary condition at the left edge of the interval

$$\psi_1 + (0{,}5u_0 + ik\Delta)\psi_0 = 2ik\Delta. \quad (9)$$

Similarly, by introducing another "dummy"grid node x_{N+1} we find the second boundary condition

$$\psi_{N+1} + (0{,}5u_N + ik\Delta)\psi_N = 0. \quad (10)$$

Now the system of equations, which includes the finite difference equations (6) and the boundary conditions (9) and (10), takes the form

$$\psi_{n-1} + u_n\psi_n + \psi_{n+1} = 0,$$

$$\psi_1 + (0{,}5u_0 + ik\Delta)\psi_0 = 2ik\Delta,$$

$$\psi_{N+1} + (0{,}5u_N + ik\Delta)\psi_N = 0.$$

The solution to equation (6) will be sought in the form

$$\psi_{n+1} = R_n\,\psi_n. \quad (11)$$

For the coefficients R_n, we find the recurrence relation

$$R_{n-1} = \frac{1}{R_n+u_n}. \quad (12)$$

For R_n, the boundary condition at the right edge of the interval is as follows

$$R_{N-1} = \frac{1}{0.5\,u_N+ik\Delta}. \quad (13)$$

Now, starting from R_{N-1} which is determined by the relation (13) using the recurrence relation (12), we will search for $R_{N-2}$and so on, moving from the $(N-1)$ - node to the node - 0, sequentially calculating R_{N-2}, R_{N-3} ... R_1, R_0, we will find all N values R_n; $(n = 0; 1; \dots; N)$.

Using the expression for R_0, we find the wave function $\psi_1, \psi_2, \dots, \psi_N$

$$\psi_0 = \frac{2ik\Delta}{R_0+0{,}5u_0+ik\Delta}. \quad (14)$$

Now, moving in the opposite direction from node 0 to the $(N-1)$ node using (6), we will sequentially find the

wave function at all the internal grid nodes $\psi_1, \psi_2, \dots, \psi_N$. Therefore, the sweep algorithm involves using the value R_{N-1} and calculating the coefficients R_n $(n = N - 2; N - 3, \dots, 0)$ using the formula (13), and then using R_0 and calculating the wave functions ψ_n; $(n = 1; 2; \dots, N)$ using the formula $\psi_n = R_{n-1}\psi_{n-1}$.

The Thomas algorithm is used for the numerical implementation of finding the transmission coefficient $\tau(E)$ of carriers through the quantum threebarrier structure and is based on the calculation formulas for the coefficients R_n (12) when they are sequentially applied from the $(N - 1)$th node to the zero node and the use of the relation (11) for the implementation of the reverse recursive process. The obtained values N for different values of the parameter ε in the interval from 0 to 10 relative units will be used to obtain the transmission coefficient according to the relation

$$\tau(E) = |\psi_N|^2. \qquad (15)$$

The obtained array for $\tau(E)$ is used for numerical calculation of specific electrical conductivity and the Seebeck coefficient according to the relations (2) and (3), as well as the power factor $P = \sigma S^2$.

Both stages of the algorithm are implemented in a single program in the computer mathematics package Maple, which are detailed in the work ([13]).

A graphical illustration of the calculation results for barriers with a height of one relative unit, $V/E_0 = 1$ and a width of $a/a_0 = 1$, i.e., one relative unit, and wells of the same depth and a width of $b/a_0 = 6$, i.e., six relative units, is shown in Figures 2, 3, and 4. The ordinate axis shows the specific conductivity in relative units σ/σ_0 the Seebeck coefficient also in relative units S/S_0, and the power factor $\sigma S^2/(\sigma_0 \cdot S_0^2)$.

3.2. An exactly solvable model for calculating the thermoelectric characteristics of nanostructured material.

For the considered problem, there exists an exactly solvable model that assumes the existence of two rectangular potential barriers with a width comparable to the thickness of the intergranular gap and a rectangular potential well with a width comparable to the grain size. The corresponding potential can be written in the following form

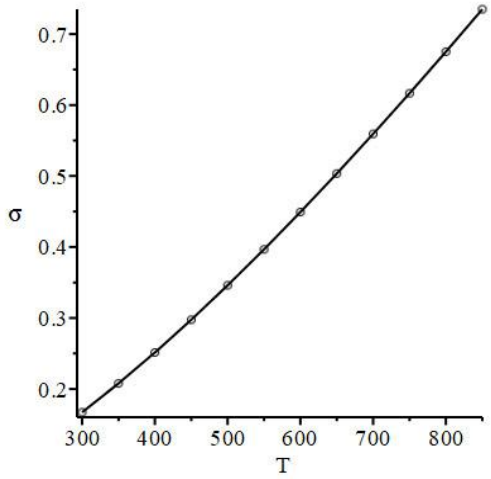

Fig. 2. The temperature dependence of the specific conductivity σ for the barrier-well-barrier structure based on the Gaussian potential.

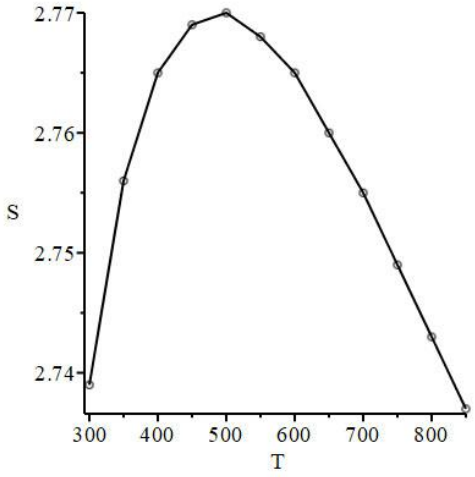

Fig. 3. The temperature dependence of the Seebeck coefficient S for the barrier-well-barrier structure based on the Gaussian potential.

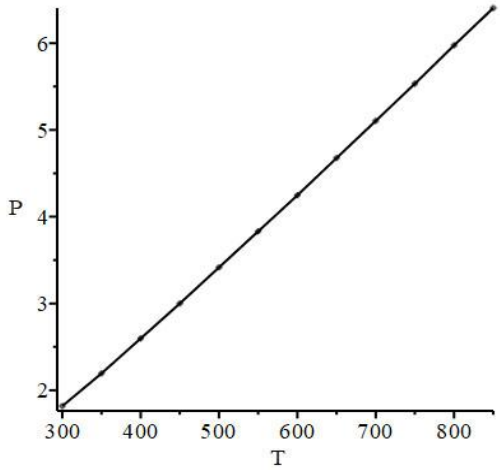

Fig. 4. The temperature dependence of the power factor $P = \sigma S^2$ for the barrier-well-barrier structure based on the Gaussian potential.

$$V(x) = \begin{cases} 0, & x < 0, \\ V_0, & 0 \le x \le a, \\ -1, & 0 \le x \le a+b, \\ V_0, & a+b \le x \le a+b+a, \\ 0, & x > a+b+a. \end{cases}$$

To obtain an exact expression for the transmission coefficient, the quantum impedance method is used [14].

The reflection coefficient for the quantum structure of a rectangular barrierwell-barrier will be

$$R = \left(2\frac{k_1^2 - k_0^2}{k_0 k_1}A_1(a) + \frac{k_2^2 - k_0^2}{k_0 k_2}A_2(b) + \frac{k_1^4 - k_0^2 k_2^2}{k_0\, k_1^2 k_2}A_1^2(a)\ A_2(b)\right)^2 \Big/ \left(4\left(1 - A_1^2 - \frac{k_1^2 + k_2^2}{k_1\, k_2}\ A_1^2(a)\ A_2(b)\right)^2 + \left(2\frac{k_1^2 + k_0^2}{k_0 k_1}A_1(a) + \frac{k_2^2 + k_0^2}{k_0 k_2}A_2(b) - \frac{k_1^4 + k_0^2 k_2^2}{k_0\, k_1^2 k_2}A_1^2(a)\ A_2(b)\right)^2\right),$$

where $A_1(a) = tan(k_1 a)$, $A_2(b) = tan(k_2 b)$.

The expression for the transmission coefficient can be found in the following way

$$\tau = 1 - R.$$

Using the obtained expression for $\tau(E)$, the specific electrical conductivity σ, the Seebeck coefficient S, and the power factor $P = \sigma S^2$ as functions of temperature are calculated using the symbolic mathematics tools in the Maple package, which are detailed in the work ([15]).

A graphical representation of the calculation results for rectangular potential barriers with a height of one relative unit, $V/E_0 = 1$ and a width of one relative unit a/a_0 , and a rectangular potential well of the same depth and a width of $b/a_0 = 8$ relative units, is shown in Figures 5, 6, and 7. As in the case based on the Gaussian potential, the ordinate axis shows the specific conductivity in relative units σ/σ_0 the Seebeck coefficient in relative units S/S_0 and the power factor $P = \sigma S^2/(\sigma_0\ S_0^2)$.

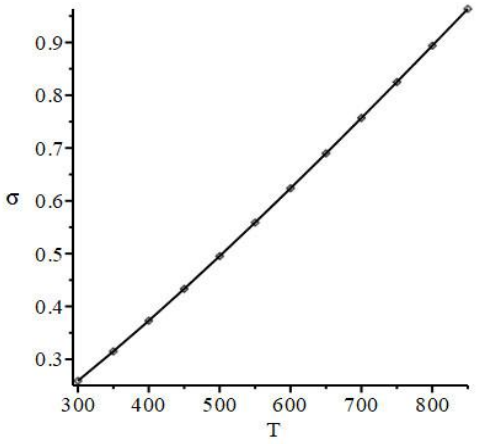

Fig. 5. The temperature dependence of the specific conductivity σ for the barrier-well-barrier structure based on rectangular potentials.

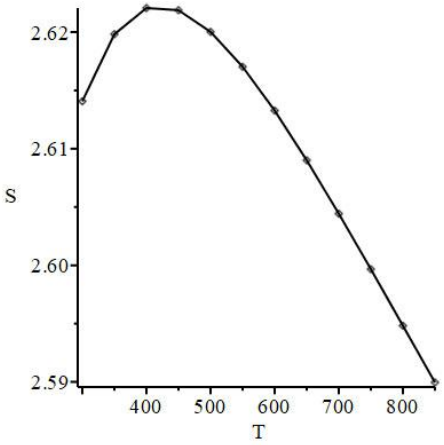

Fig. 6. The temperature dependence of the Seebeck coefficient S for the barrier-well-barrier structure based on rectangular potentials.

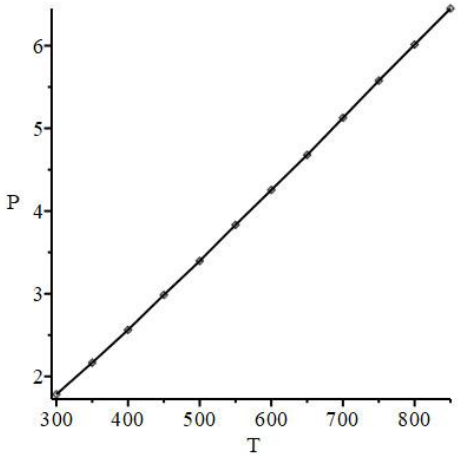

Fig. 7. The temperature dependence of the power factor $P = \sigma S^2$ for the barrierwell-barrier structure based on rectangular potentials

3.3. The model of a nanostructured thermoelectric material is based on the Poschl-Teller potential.

Let's consider another example of a barrier-well-barrier structure, this time based on the Poschl-Teller potential. This potential is similar in shape to the Gaussian potential but has a number of interesting features. In particular, both for the potential barrier and for the well, analytical expressions for the transmission coefficients $\tau(E)$ are known for a given potential, and under certain values of its parameters, the Poschl-Teller potential becomes reflectionless. Now, the potential of the nanostructure will be described by the function

$$V(x) = \frac{1}{\cosh{(3(x-1))^2}} - \frac{1}{\cosh(x-5)^2} + \frac{1}{\cosh(3(x-9))^2}. \quad (17)$$

which describes a Poschl-Teller type barrier with a half-width of one relative unit centered at the point $x/x_0 = 1$, a quantum well also of the Poschl-Teller type with a width of six relative units centered at the point $x/x_0 = 5$, and a Poschl-Teller type barrier with a half-width of one relative unit centered at the point $x/x_0 = 9$. The height of the potential barriers and the depth of the potential well are both equal to one relative unit. The algorithm for calculating the transmission coefficient, specific conductivity, Seebeck coefficient, and power factor is implemented using the program employed for the corresponding calculations for the barrier-well-barrier quantum structure based on the Gaussian potential. A graphical illustration of the calculation results for barriers with a height of one relative unit, a half-width $a/a_0 = 1$, i.e., one relative unit, and a well of the same depth and a $b/a_0 = 6$, i.e., six relative units, is shown in Figures 8, 9, and 10.

IV. Calculation results

From the analysis of the calculation results for all three types of barrierwell-barrier quantum structures, it follows that in all cases the values of the relative Seebeck coefficient are close. The difference between them does not exceed 15 percent. Therefore, the presence of barriers and wells is crucial for the increase of the thermoelectric coefficient, and changing their shape does not lead to significant changes.

Using the developed program, a study of the temperature dependencies of the specific electrical conductivity σ, the Seebeck coefficient S, and the power factor $P = \sigma S^2$ on the height of the intergranular barriers and the distance between them, i.e., the size of the nanograins, was conducted.

The calculations showed that with an increase in the height of the barrier, the specific conductivity

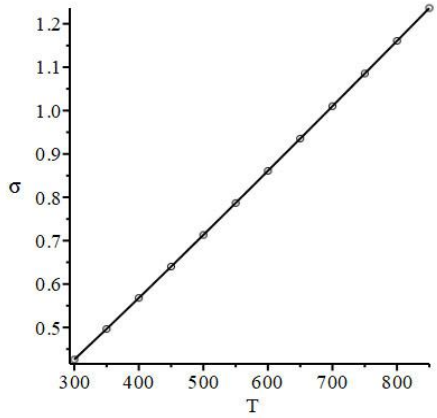

Fig. 8. The temperature dependence of the specific conductivity σ for the barrier-well-barrier structure based on the Poschl-Teller potential.

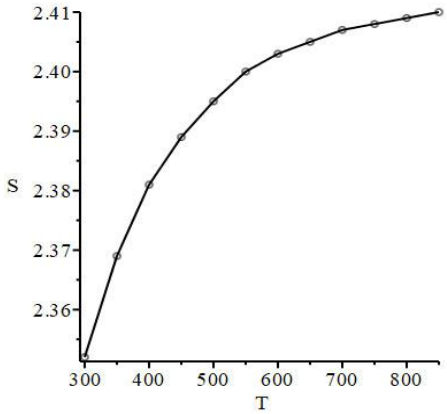

Fig. 9. The temperature dependence of the Seebeck coefficient S for the barrier-well-barrier structure based on the Poschl-Teller potential.

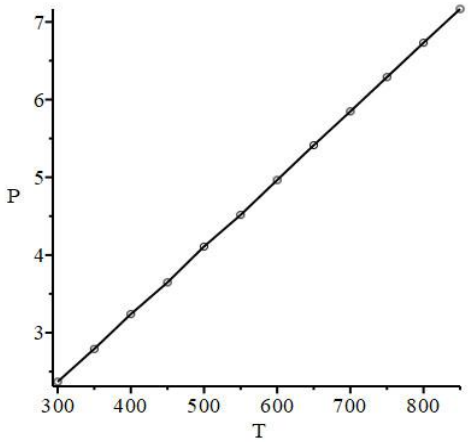

Fig. 10. The temperature dependence of the powerσS^2 for the barrierwell-barrier structure based on the Poschl-Teller potential.

significantly decreases, particularly with a twofold increase in the height of the barrier, the decrease in specific conductivity is also close to two.

A similar behavior is observed in the dependence of specific conductivity on the width of the barrier. From the graphs shown in Figures 11 and 12, it can be seen that with oth a twofold increase in the height of the barrier and an increase in its halfwidth from approximately ~0.3 to approximately ~0.7, the Seebeck coefficient increases by approximately 20 percent.

However, changing the distance between the barriers, i.e., the width of the well, has little effect on the thermoelectric characteristics of the proposed quantum structure. Figure 13 shows a graph of the transmission coefficient dependency on the energy of the incident particle $\tau(E)$, where at least six resonance peaks are observed. However, the calculation of the eigenvalues of energy in the mentioned structure using the developed program, which determines the eigenvalues by diagonalizing the matrix formed from the coefficients at the values of the wave function at the grid nodes, gives only three values. Also, the correspondence between the resonance energies and the bound state energies is incomplete. This discrepancy confirms the fact that the number of resonance energies and the number of stationary states in the quantum well are not mutually uniquely determined.

As can be seen from the graphical representation of the calculation results of the temperature dependence of the Seebeck coefficient S for four different widths of the potential well b, specifically for $b = 8, b = 6, b = 4$, and $b = 2$, the change in the Seebeck coefficient for $b = 8$ when $\tau(E)$ has five resonance peaks to the case when resonance states are completely absent at $b = 2$ does not exceed 4 percent. Such behavior of the Seebeck coefficient is obviously related to the fact that the function $\tau(E)$ in the expressions for conductivity and thermoelectric electromotive force is included in the integral. Therefore, the presence of resonance tunneling slightly changes both the Seebeck coefficient and the power factor of the nanostructured material.

It should be noted that the obtained values of the thermoelectric characteristics and their behavior with changing temperature and parameters of the quantum structure are consistent with the results obtained by other authors, in particular [3], [7], [10], [11]. For the model described by the Poschl-Teller potential for both the barrier and the well, analytical expressions for the

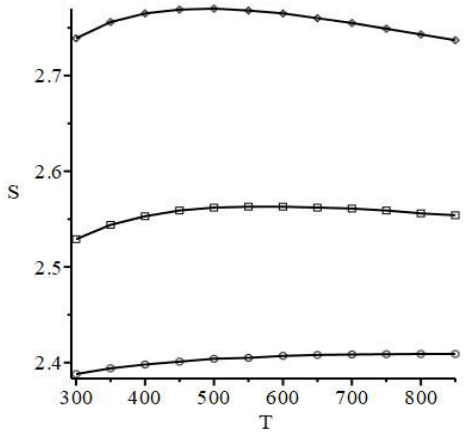

Fig. 11. The temperature dependence of the Seebeck coefficient as a function of barrier height: ” ◦ ” - for $V0 = 1$, ▫ - for $V0 = 1{:}5$, ”◇” - for $V0 = 2$.

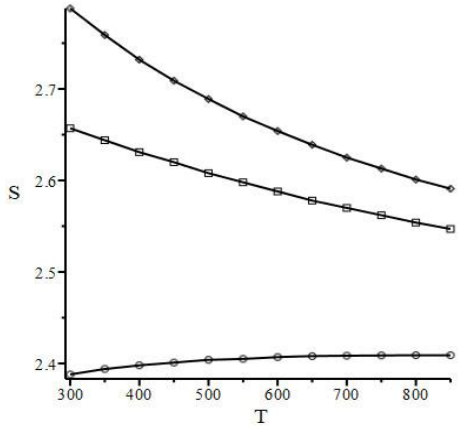

Fig. 12. The temperature dependence of the Seebeck coefficient as a function of barrier width: ” ◦ ” - for a half-width of $1{=}3$, ▫ - for a half-width of $0{:}5$, ”◇” - for a half-width of $1{=}\sqrt{2}$.

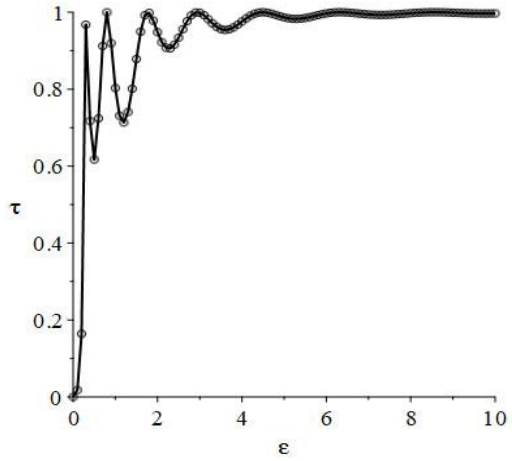

Fig. 13. The transmission coefficient for the barrier-well-barrier structure based on the Poschl-Teller potential with a well width of six relative units.

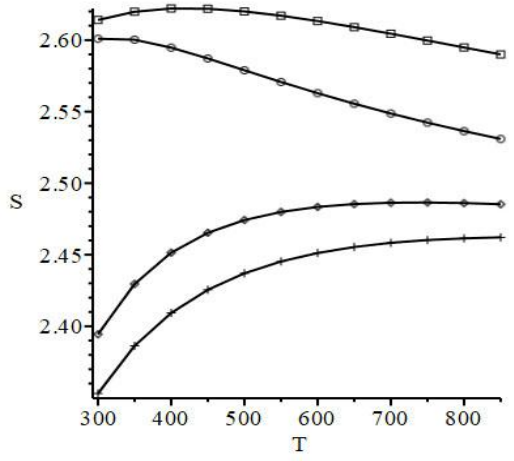

Fig. 14. Thermoelectric EMF of a triple-barrier structure as a function of temperature for well widths b: $b = 2$ - ◦, $b = 4$ - ”◇”, $b = 6$ - ” + ”, $b = 8$ - ▫.

Table 1.

Comparison of the results of the numerical calculation of the Seebeck coefficient for the model based on the Peschl-Teller potential – SPT with the results of the calculation using the approximation $\tau(E) = \tau_1(E) \cdot \tau_2(E) \cdot \tau_3(E)$ – S_A from the temperature T

1	2	3	4	5	6	7	8
TK	300	350	450	600	700	800	900
SA	2:24	2:28	2:31	2:33	2:33	2:32	2:31
SP T	2:35	2:37	2:39	2:4	2:41	2:41	2:31

transmission coefficients $\tau(E)$ are known [16]. In particular, the transmission coefficient through the barrier

$$V(x) = \frac{\hbar^2}{2ma^2}\frac{U_0}{cosh^2\left(\frac{x}{a}\right)}.$$

with the condition $\frac{2ma^2U_0}{\hbar^2} < 1$, is given by the expression

$$\tau(E) = \frac{sinh^2(\pi ka)}{sinh^2(\pi ka)+cosh^2\left(\pi\sqrt{\frac{1}{4}-\frac{2ma^2U_0}{\hbar^2}}\right)},$$

with the condition $\frac{2ma^2U_0}{\hbar^2} > 1$, is given by the expression

$$\tau(E) = \frac{sinh^2(\pi ka)}{sinh^2(\pi ka)+cosh^2\left(\pi\sqrt{\frac{2ma^2U_0}{\hbar^2}-\frac{1}{4}}\right)},$$

with the condition $\frac{2ma^2U_0}{\hbar^2} = \frac{1}{4}$, is given by the expression

$$\tau(E) = tanh(\pi ka).$$

In the given expressions

$$k = \sqrt{\frac{2mE}{\hbar^2}}.$$

If the potential well is defined using the modified Poschl-Teller potential in which two bound states exist

$$V(x) = -\frac{\hbar^2}{2ma^2}\frac{U_0}{cosh^2\left(\frac{x}{a}\right)} = -\frac{6}{cosh^2\left(\frac{x}{a}\right)},$$

which belongs to the category of so-called reflectionless potentials, and therefore, the corresponding transmission coefficient is one, which significantly simplifies the calculation of thermoelectric characteristics related to tunneling transport mechanisms.

In the general case, the potential for the modified Poschl-Teller well has the following form

$$V(x) = -\frac{\hbar^2}{2ma^2}\frac{\lambda(\lambda-1)}{cosh^2\left(\frac{x}{a}\right)},$$

and the transmission coefficient for it is given by

$$\tau(E) = \frac{sinh^2(\pi ka)}{sin^2(\pi\lambda)+sinh^2(\pi ka)}.$$

If the expression for the transmission coefficient of the barrier-well-barrier quantum structure uses the approximation $(E) = \tau_1(E)\,\tau_2(E)\,\tau_3(E)$, where $\tau_1(E)$ is the transmission coefficient of the first barrier, $\tau_2(E)$ is the transmission coefficient of the well, and $\tau_3(E)$ is the transmission coefficient of the third barrier, which is an approximatio (Table 1).

Comparison of the numerical calculation results with the results obtained using the approximated expression for $\tau(E)$ showed that the deviation between the results does not exceed ten percent, making the applied approximation a convenient tool for quick prediction of the thermoelectric characteristics of the material with certain parameters of the Poschl-Teller potential.

Conclusions

A one-dimensional model of a nanostructured thermoelectric material has been proposed, in which the nanograin is modeled by a potential well, and the intergranular boundaries are modeled by potential barriers. The well and barriers are modeled by the Gaussian potential with different parameters. The modeling process is implemented as a program developed on the Maple computer mathematics platform. Using the developed program, the temperature dependencies of the specific conductivity σ, the Seebeck coefficient S, and the power factor $P = \sigma S^2$ have been calculated and their graphical illustration is provided.

It has been shown that with an increase in the height and width of the barriers, the conductivity of the quantum structure decreases, while the Seebeck coefficient increases. At the same time, the power factor $P = \sigma S^2$ decreases with an increase in the height of the barriers, and changing the istance between the barriers, i.e., the width of the well, has little effect on the thermoelectric characteristics of the proposed quantum structure.

For the exact solvable case when the barriers and the well are rectangular, the method of quantum impedance has been used to obtain an analytical expression for the particle transmission coefficient. Using symbolic mathematics in the Maple package, calculations of the temperature dependence for specific conductivity σ, the Seebeck coefficient S, and the power factor $P = \sigma S^2$ have been carried out.

It has been shown that increasing the height of the barriers causes a decrease in specific conductivity and an increase in the Seebeck coefficient. It was found that changing the width of the potential well slightly changes the Seebeck coefficient, and the power factor remains almost constant. For the proposed model, the effect of resonance tunneling of particles through the barrier-well-barrier quantum structure on the thermoelectric characteristics of the nanostructured material was considered. It was found that the presence of resonance tunneling has little effect on the Seebeck coefficient and

the power factor.

For the modified Poschl-Teller potential, with certain parameter values, it is possible to obtain analytical expressions for the transmission coefficients τ of the well and barrier. Assuming that the transmission coefficient of the barrier-well-barrier system is equal to the product of the transmission coefficients of the components of this system, it has been shown that the difference between the numerical and analytical calculations is practically non-existent. This result indicates the feasibility of using this approach (model) for a quick analysis of the thermoelectric parameters of a nanomaterial based solely on relatively simple analytical expressions.

Based on the proposed one-dimensional model of a nanostructured thermoelectric material, calculations of thermoelectric parameters (Seebeck coefficient, specific electrical conductivity, and thermoelectric power) have been carried out. It was found that the numerical values of thermoelectric power practically do not depend on the type of chosen potential (Gaussian, Poschl-Teller, or rectangular) and, with the same height and width, differ by no more than 15

Based on the generalization of the obtained results, it can be concluded that with variations in the energy parameters, particularly the height and width of the potential barriers of the nanostructured material model, achieving a significant qualitative improvement in thermoelectric power P is difficult. However, quantitative optimization of the power factor magnitude with variations in the height and width of the barriers can be achieved at the level of 10-15.

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Модель для розрахунку термоелектричних властивостей наноструктурованого матеріалуі

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Для моделі бар'єр-яма-бар'єр наноструктурованого термоелектричного матерілу, яка базується на потенціалах Гаусса, Пешль-Теллєра та прямокутних бар'єрах і ямі, виконано розрахунки термоелектричних характеристик. Для квантових структур бар'єряма-бар'єр на базі потенціалів Гаусса і Пешль-Теллєра розроблена програма для розрахунку термоелектричних характеристик в основі якої Thomas algorithm для розрахунку коефіцієнта проходження частинок через квантову структуру та чисельного інтегрування виразів для питомої електропровідності та коефіцієнта термое.р.с. із відповідною графічною ілюстрацією одержаних результатів. Програма розрахунків реалізована на платформі комп'ютерної математики Maple. Для квантової структури на базі прякутних потенціалів із застосуванням методики квантового імпедансу, одержано вираз для коефіцієнта проходження частинок через таку структуру та застосовано його для розрахунку засобами символьної математики пакету Maple питомої провідності, коефіцієнта Зеебека та фактора потужності. Враховано вплив резонансного тунелювання частинок через запропоновану трибар'єрну структуру на її термоелектричні характеристики. Подано аналіз одержаних результатів розрахунків.

Ключові слова: квантовий тунельний механізм термоелектричних явищ, модель наноструктурованого матеріалу, коефіцієнт Зеєбека, коефіцієнт потужності.