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Thermoelectricity of Nanostructures Based on Compounds of Lead Telluride

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The thermoelectric parameters have been investigated depending on the thickness of the layer of nanostructures PbTe doped by Bi. Based on the theoretical model of quantum well (QW) with infinitely high walls, it is demonstrated that this model explains nonmonotonous behaviour of the Seebeck coefficient S and electric conductivity σ with the change of the well width.

Keywords: Nanostructures, Thermoelectricity, Electrical properties.

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1. INTRODUCTION

Recently, in the process of creating highly efficient thermoelectric materials, the research in the low-dimensional structures has been intensified [1]. The reducing of the material dimension creates the conditions for observing the phenomenon of quantum-size effect, which increases the density of states near the Fermi energy. This allows to sufficiently save high electrical conductivity σ at the relatively low Fermi energy E_F, where there are high values of the Seebeck coefficient S.

The behavior of thermoelectric parameters (the electrical σ and thermal conductivity k, the Seebeck coefficient S) in bulk materials is usually described in terms of electronic and phonon properties that change greatly with the reducing of the sample size below ~ 100 nm, where the quantum effects become more significant. The spatial restriction of the acoustic phonons and the appropriate modification of the group velocity leads to the increase in phonon relaxation rate and results in the decrease of lattice thermal conductivity k_L [2]. Besides, the nature of interactions between the charge carriers changes greatly. The theoretical calculations associated with the estimation of these effects on the transport coefficients are usually performed within the framework of size quantum limit, which is based on the simplification that electrons occupy only the lowest sub-bands. In such an approach, consideration of the multiple sub-band structure of quantum well can lead to nonmonotonous changes of various kinetic parameters such as mobility μ, the Seebeck S and the Hall coefficients R_H [3].

The aim of this study is to verify the expediency of using the model of infinitely deep rectangular QW for compound PbTe: Bi, grown on substrates glass-ceramic.

2. THEORETICAL MODEL AND RESULTS OF CALCULATIONS

For the quantum well with high walls, the electrons are confined in the direction of *OZ*, but in the *X*- and *Y*-directions their movement is autonomous. The electronic wave function and energy eigenvalues in terms of parabolic energy bands are determined by equations [3]:

$$\psi = (2/\Omega)^{1/2} \exp(ik_x x + jk_y y)\sin(n\pi z/d) \quad (1)$$

$$E = \frac{\pi^2\hbar^2}{2m_z^* d^2} n^2 + \frac{\hbar^2 k^2}{2m_p^*}, \quad (2)$$

where $k^2 = k_x^2 + k_y^2$, m_z^* – effective mass of electron along confinement direction; $m_p^* = \sqrt{m_x^* m_y^*}$, m_x^*, m_y^* – effective masses of electron along the x and y axes, Ω – total volume of the layer, d – well width, n – quantum number that obtains values of natural numbers.

At this condition it is possible to write down the expressions for the Seebeck coefficient and electric conductivity as:

$$S = \frac{k_B}{e}\left[\frac{E_F}{k_B T} - \frac{A_1 - A_2}{A_3}\right], \quad (3)$$

$$\sigma = \frac{1}{2\pi d}\frac{2k_B T}{\hbar^2}\sqrt{\frac{m_x^*}{m_y^*}} e^2 \tau_0 A_3, \quad (4)$$

where:

$$A_1 = \left(\sum_{n=1}^{E_n \le E_F} \int_0^\infty \left(-\frac{\partial f_n}{\partial x}\right) dx\right), \quad (5)$$

$$A_2 = \left(\sum_{n=1}^{E_n \le E_F} E' \int_0^\infty x\left(-\frac{\partial f_n}{\partial x}\right) dx\right), \quad (6)$$

$$A_3 = \left(\sum_{n=1}^{E_n \le E_F} \int_0^\infty x\left(-\frac{\partial f_n}{\partial x}\right) dx\right). \quad (7)$$

The Fermi distribution function has a known form:

$$f_n = \frac{1}{e^{x-\eta_n} + 1}, \quad (8)$$

where $x = \varepsilon/k_B T$ – reduced carrier energy, $\eta_n = \xi - E_n'$. Here $\xi = E_F/k_B T$ and $E_n' = E_n/k_B T$.

It is possible to estimate the relaxation time in (4) using the n-type carriers mobility μ in a bulk sample [4]:

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$$\mu = e\tau_0 / m\,, \tag{9}$$

The Fermi energy value can be expressed through the well width (d) and the concentration of carrier in the conduction band [5]

$$E_F = \varepsilon_1 \frac{(n_0+1)(2n_0+1)}{6} + \frac{\pi\hbar^2}{m^*}\frac{n_{el}}{n_0}d\,, \tag{10}$$

where ε_1 – the first quantized level, when $n = 1$; $n_0 = [(E_F/\varepsilon_1)^{1/2}]$ – the effective mass of carriers, n_{el} – electronic concentration.

If the Fermi lever coincide with the bottom of the band n_0, then $E_F(d_0) = \varepsilon_1 n_0^2$. At such widths $(E_F(d_0)/\varepsilon_1)^{1/2}$ is an integer. Putting this value in (10) for d_{n0} we get:

$$d_{n_0} = d_0 n_0 \left[1 - \varepsilon_1 \frac{(n_0+1)(2n_0+1)}{6n_0^2}\right]^{1/3}, \tag{11}$$

where $d_0 = (\pi/2n_{el})^{1/3}$. A number n_0 at this width is a whole part from the result of decision of equation (11) relatively to n_0 when $d_{n0} = d$.

The influence of doping level by Bi on PbTe can be estimated through the proper change of effective mass in (10) using an empiric formula, what have been gotten as a result of approximation of experimental dependence of effective mass on an electronic concentration [6]:

$$\frac{m^*}{m_0} = 0{,}111 \cdot 10^{-6} \cdot n_{el}^{\frac{1}{3}}\,, \tag{7}$$

де m_0 – the mass of electron, n_{el} – an electronic concentration in units of cm^{-3}.

The account of the Fermi energy d-dependence in formulas (3)-(8), and also the effective mass z-component d-dependence in expressions (5)-(8) allow to get the proper dependences of Seebeck coefficient S and electric conductivity σ on the width of quantum well PbTe:Bi. Amount of levels below the Fermi energy is determined by d-dependences of effective mass and E_F, and also by well width d. Calculation procedure took into account both the change of Fermi energy and the change of amount of levels below it at the change of well width. Also, at the calculation of conductivity it was assumed on a formula (4), that $m_x^* = m_y^*$.

Using the described higher theoretical model for description of the behaviour of thermoelectric coefficients in the nanostructures PbTe:Bi at 300 K the quantum well width in a theoretical model was considered to be equal to the condensate thickness in experimental dependences of the proper parameters. The resulting dependences of thermoelectric coefficients on the well width PbTe:Bi are characterized by an unmonotonous oscillation behaviour (Fig. 1). Thus the calculating values are well enough conformed to proper experimental dependences.

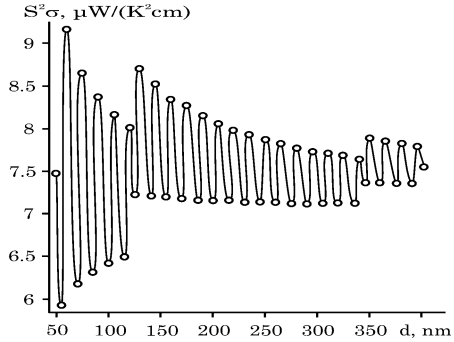

Fig. 1 – Theoretical dependences of the Seebeck coefficient (a), electric conductivity (b) and thermoelectric power coefficient $S^2\sigma$ on the width of PbTe:Bi quantum well in a model of infinitely deep potential well at T = 300 K

3. CONCLUSIONS

1. The analysis of experimental dependences for thermoelectric coefficients on the thickness of nanostrucutures PbTe:Bi on a class-ceramic at 300 K have been done. It is discovered that they are characterized by an unmonotonous oscillation behaviour.
2. In the model of quantum well with infinitely high walls the dependences of Fermi energy and effective mass on the well width are calculated. On their basis it was investigated the character of oscillations period change for the density of states with well width growth.
3. On the basis of correlations of Fermi energy and effective mass with the well width there were built d-dependences of Seebeck coefficient, electric conductivity and thermoelectric power coefficient. It was shown that the theoretical d-dependences conform to the experimental.

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