

QUANTUM-SIZE EFFECTS IN NANOSTRUCTURES ON THE BASE OF COMPOUNDS IV-VI

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ABSTRACT

Thickness dependences of kinetic parameters of quantum wells (QWs) based on IV-VI compounds show non-monotonic oscillatory behavior that is associated with size quantization due to carrier movement restrictions in one direction.

In work on basis of theoretical model of rectangular quantum well with infinitely high barriers we investigated the dependences of thermoelectric parameters on nanostructures thickness of compounds IV-VI (PbTe, PbSe, PbS, SnTe). It was shown, that in such structures it has place nonmonotonous, oscillation change of thermoelectric coefficients with well width. Thickness dependence of the Seebeck coefficient S , based on model of QW with infinitely high walls, are characterized by breaks with some period. For quantum wells SnTe it was found good agreement between the values of theoretical and experimental oscillating amplitude in dependence $S(d)$.

Shown, that values Δd_{exp} of oscillations period are equal to QW thickness d_{min} , when the bottom of lowest subband coincides with the Fermi energy E_F . This thickness d_{min} was explained as the minimum QW thickness, when quantum size effects are the main factor, that determines the nonmonotonous behaviour in thickness dependencies of thermoelectric parameters of the relevant structures. At smaller thicknesses important factor, affecting the change of kinetic parameters with thickness, is the phenomenon of percolation. It is shown that the percolation transition changes the value of the concentration of main type carrier in nanostructure, thereby changing the Fermi energies and hence the period of oscillations. Thus, the sudden change of concentration of the main type carrier results in a sharp change in oscillations period of thickness dependence of kinetic parameters.

Key words: nanostructures, quantum-size effects, thermoelectricity

INTRODUCTION

In the process of creating highly efficient thermoelectric materials at recent times it has place an intensification of research in low-dimensional structures [1,2]

The behavior of thermoelectric parameters (electrical and thermal conductivity k , Seebeck coefficient S) in bulk materials is usually described in terms

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of electronic and phonon properties that change greatly with reducing of sample size below the micrometer range, where quantum effects become more significant. Spatial restriction of acoustic phonons and the corresponding modification of group velocity leads to an increase in phonon relaxation rate, resulting in decrease lattice thermal conductivity k_L . Also the nature of interactions between particles changes greatly.

Electronic restriction by reducing sample size leads to increased energy gap E_g , which in turn affects the transport properties. By quantization the conduction band density of states changes abruptly with change of energy. Depending on probability amplitude electrons can be found in any sub-bands ($E_1, E_2, \dots E_n$), with a certain probability hop from one band to another nearest band and occupy levels up to the Fermi energy.

THEORETICAL MODEL

For quantum well with high walls, electrons are confined in the direction of oz , but in the x - and y -directions their movement is free.

In case of quantum well thermoelectric transport coefficients can be obtained from Boltzmann equations, which are written under the assumption that in steady state electronic distribution function remains constant and changes only by external forces and fields. Then system of electrons returns to equilibrium through various relaxation processes with characteristic relaxation times. for quasi-two dimensional system it can be written [3]:

$$S = \frac{E_F}{eT} + \frac{1}{eT} \frac{\Gamma^2}{\Gamma^1}. \quad (1)$$

Transport coefficient Γ is defined by semi-classical approach, in which particles are confined in one-dimensional box. Thermal gradient and electric field are directed along ox -axis. Then:

$$\Gamma^1 = -\zeta^{(0)}, \quad (2)$$

$$\Gamma^2 = \zeta^{(1)}, \quad (3)$$

where:

$$\zeta^{(s)} = \frac{2T}{\pi a} \sqrt{\frac{m_y^*}{m_x^*}} \frac{1}{\hbar^2} \sum_{n=1}^{E_n \leq E_F} \int_0^\infty E^s \tau \varepsilon \left(\frac{\partial f}{\partial \varepsilon} \right) d\varepsilon. \quad (4)$$

Here f - Fermi distribution function, $\varepsilon = E - E_n$, τ - relaxation time in the case of scattering by acoustic phonons.

RESULTS AND DISCUSSION

Basing on experimental data [4,5,6,7], which show nonmonotonous, oscillatory character for dependences of Seebeck coefficient on the condensate thickness, it is natural to assume that such behavior is due to quantization of

carriers energy by restriction their movement in the potential well. Increasing well width on the value of half Fermi wavelength leads to new sub-band below the Fermi energy. At width when the new band is filled in the density of states there is a jump, which leads to oscillating behavior.

Using the above theoretical model to describe behavior of Seebeck coefficient in nanostructures PbS, PbSe, PbTe, SnTe at 300 K, quantum well width in the theoretical model was considered equal to the thickness of condensate in experimental dependences $S(d)$. Calculations were carried out for different well widths at given values of Fermi energy, which is a function of concentration and temperature. Fig. 1 shows d -dependences of Seebeck coefficient for the QW PbS, PbSe, PbTe (a) and SnTe (b) with experimentally determined oscillation period Δd_{exp} . It is seen that dependences of Seebeck coefficient S on well width are characterized by discontinuities with some period. Note that procedure of calculation the dependences $S(d)$ for compounds IV-VI (fig. 1) takes into account different number of filled bands for various well widths at fixed Fermi energy.

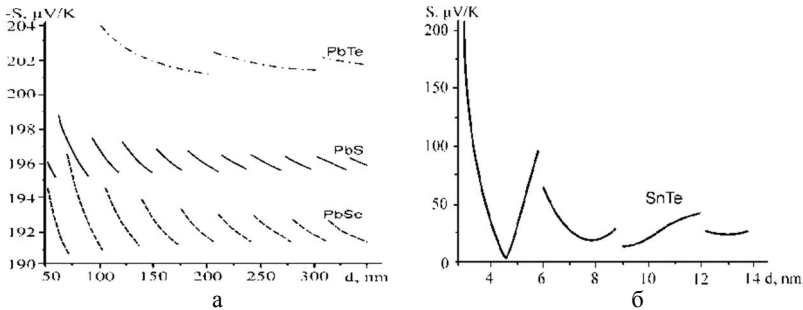


Fig. 1 – Dependence of Seebeck coefficient on the width d of QW PbS, PbSe, PbTe (a) and SnTe (b) in the model infinitely deep potential well

In considered approach the experimental value of oscillation period is equal to minimum QW width d_{min} , from which quantum-size effects are the main factor that conditions nonmonotonous change of thickness dependencies TE-parameters in relevant structures.

Evaluating value of Fermi energy on the basis of experimentally determined values of carrier concentration it is possible to compare received oscillation periods with its experimental values. Thus in contrast to PbS and PbTe QW for QW PbSe and SnTe it is obtained a good agreement with experiment: PbSe: $\Delta d_{\text{theor}} = 27$ nm and $\Delta d_{\text{exp}} \approx 35$ nm; SnTe: $\Delta d_{\text{theor}} = 3$ nm and $\Delta d_{\text{exp}} \approx 2.9$ nm [4,5,6,7].

Assuming that percolation processes leads to the extrema points displacement of experimental dependence $S(d)$ in comparison with theoretical, we can

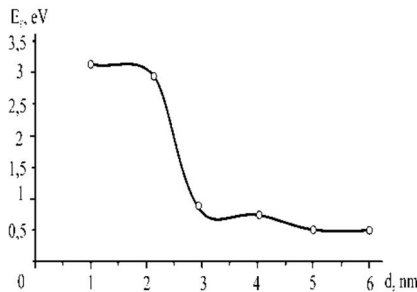


Fig. 2 – Dependence of Fermi energy on SnTe well width, obtained by comparing the theoretical dependences $S(d)$ for different oscillation periods with experimental

note a decrease their influence with increase SnTe thickness.

On the other hand, if percolation processes alter the main type carrier concentration in nanostructure, thereby changing Fermi energy and hence oscillation period, then abrupt change in carrier concentration would lead to abrupt changes in oscillation period of d -dependence of Seebeck coefficient. Since the oscillation period is associated with Fermi energy, it is possible to construct the dependence $E_F(d)$ (fig. 2). Fig. 2 shows that with changing well

CONCLUSIONS

1. Shown that dependences of Seebeck coefficient on width of quantum well with infinitely high walls for structures based on IV-VI compounds are characterized by discontinuities with some period.

2. Based on experimentally determined oscillation period Δd_{exp} of the thickness dependences of Seebeck coefficient Fermi energy values are determined in QW structures of compounds IV-VI.

3. Shown that oscillation period value Δd_{exp} of quantum well is equal to the width of QW d_{min} , where the bottom of lowest sub-band coincides with Fermi energy E_F . We have given to the width d_{min} the content of minimum QW width from which quantum-size effects are the main factor that determines non-monotonous change of thickness dependencies for thermoelectric parameters in corresponding nanostructures.

4. For QW SnTe it was found good agreement between theoretical and experimental values of oscillation amplitude in dependence $S(d)$.

5. Reducing the value of difference between the experimental and theoretical extremum points with increasing SnTe QW width is explained by the reducing of the percolation phenomena impact in such growth.

6. For SnTe nanostructures shown that dependences $S(d)$ with different oscillation periods are in good agreement with experiment at different intervals of change the condensate thickness. Thus the dependence of Fermi energy on the

well width is received. Revealed a sharp change of Fermi energy in the range from 2 to 3 nm.

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