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THERMOPOWER IN SEMICONDUCTOR SUPERLATTICES AT SCATTERING OF CURRENT CARRIERS BY PHONONS AND POINT DEFECTS

In the quasi-classical one-miniband approximation, the thermopower of semiconductor superlattices (SL) is investigated in the case of arbitrary statistics and at scattering of charge carriers by acoustic phonons, point defects, and nonpolar optical phonons, taking into account the change in the relaxation time as compared to bulk materials. An analytical dependence of the thermopower on the reduced width of the conduction band β in the direction of the superlattice axis is established. It is shown that the thermopower of the superlattice increases with an increase in the width of the conduction miniband, asymptotically approaching the limiting value at $\beta \geq 10$. Bibl. 17, Fig. 3.

Key words: Seebeck coefficient, superlattice figure of merit, thermoEMF.

Formulation of the problem.

The development of modern technique and technology is closely related to the search for new sources of energy, primarily electrical. The main requirement is to increase the generation power.

However, at the present time, additional conditions are coming to the fore: energy must be produced by environmentally friendly renewable sources that are not related to carbohydrates. Thermoelectric energy is one of the promising, and in some cases the only possible way to directly convert thermal energy into electricity. A significant limitation of thermoelectric energy conversion is the relatively low efficiency of conversion of thermal energy into electricity - from 3% to 8% [1].

The efficiency of thermoelectric conversion is determined by the ratio

$$\eta = \frac{\Delta T}{T_1} \frac{\sqrt{1+ZT}-1}{\sqrt{1+ZT}+1}, \tag{1}$$

where $\Delta T = T_1 - T_2$, $T = (T_1 - T_2)/2$, T_1 is heater temperature, T_2 is refrigerator temperature,

$$Z = \frac{\alpha^2 \sigma}{\kappa_e + \kappa_{ph}}, \tag{2}$$

is figure of merit of thermoelectric material, α is the Seebeck coefficient, σ, κ and κ_{ph} are coefficients of electric conductivity, electron and lattice thermal conductivity.

Analysis of recent research and publications.

High-efficiency thermoelectric energy converters require a large thermoelectric figure of merit, which for bulk materials has approached the limit value $ZT = 1$ [2]. However, low-size systems can overcome this limit. In [3-5], it was shown that the thermoelectric figure of merit of superlattices (SL) with rather narrow quantum wells (QWs) can significantly exceed the figure of merit of bulk semiconductor samples, the composition of which is similar to that of the SL material.

In this regard, special attention is paid to the study of transport phenomena in semiconductor superlattices. In particular, a large number of theoretical [6-9] and experimental [10,11] works are devoted to the study of thermopower. Superlattices include plane-layer crystals of transition metal dichalcogenides and their compounds, A_3B_6 semiconductors, polytypic semiconductor compounds, and others [11 – 13].

In [3 – 5], using a simple parabolic dispersion law in the one-miniband approximation, it was shown that in 2D structures a significant increase in thermopower is possible in comparison with 3D structures. It was assumed that dimensional quantization does not lead to a change in the relaxation time and carrier mobility in the direction perpendicular to the plane of the layers, as compared to bulk materials. The increase in the thermopower was associated only with an increase in the density of quantum states near the edges of dimensional quantization bands. The thermopower of SL with the use of a quasi-two-dimensional energy spectrum in the approximation of the relaxation time tensor for scattering of current carriers by phonons of various types using the cosine dispersion law and degenerate statistics was studied in [9]; however, the effect of the width of the conduction miniband on the magnitude of the thermopower in the direction of the SL axis was not considered.

The purpose of this work is to study the thermopower of semiconductor superlattices in the quasi-classical one-miniband approximation at scattering of charge carriers by acoustic phonons, point defects, and nonpolar optical phonons with arbitrary statistics and taking into account the change in the relaxation time in *2D* structures compared to bulk materials.

Formulation of the problem

Presentation of the main material. In semiconductor superlattices, in addition to the periodic potential of the crystal lattice, there is an additional one-dimensional potential, the period of which significantly exceeds the lattice constant. The presence of the potential of the superlattice significantly changes the energy spectrum, due to which it is possible to arbitrarily change its band structure. The physical properties of semiconductor SL are determined by their electronic spectrum. While the movement of current carriers in the direction perpendicular to the SL axis is almost free and corresponds to movement over a wide conduction band, the movement along its *0z* axis is limited.

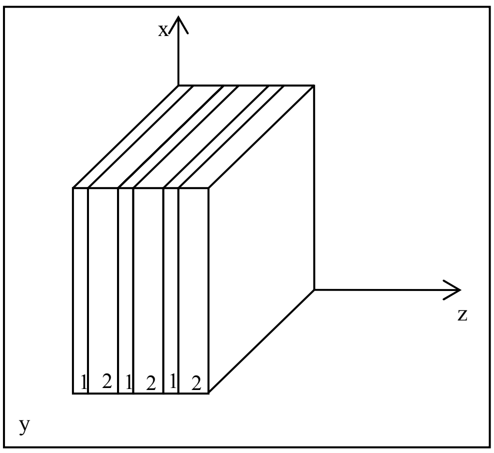

Fig.1. Schematic structure of a semiconductor superlattice. 1 - GaAs layer. 2 - AlAs layer.

In this direction, the electronic spectrum will have a miniband character. In the case of sufficiently narrow layers, which are quantum wells for electrons, all electrons will be located near the bottom of the lower miniband of dimensional quantization.

Within the framework of quasi-classical approximation

$$2\varepsilon_0 >> \hbar/\tau_{2D},\ eE_0,\ a\nabla_z k_0 T, \tag{2}$$

the dispersion law for electrons in the lower SL miniband looks like [13]

$$\varepsilon(\vec{k}) = \frac{\hbar^2 k_\perp^2}{2m_\perp} + 2\varepsilon_0(1-\cos k_z a) \tag{3}$$

where $k_\perp = (k_x^2 + k_y^2)^{1/2}$, and k_z are the transverse and longitudinal to SL axis components of quasi-wave vector, $m_\perp$ is transverse effective mass close in value to the effective mass m^* of electrons of a semiconductor forming SL, a is SL period, $2\varepsilon_0$ is the width of the conduction band of SL in the direction k_z.

The longitudinal component of the relaxation time tensor of the electron gas in SL is written in the form [15]

$$\tau_{2D} = \frac{2\sqrt{2m_\perp k_0 T}}{3\pi\hbar} a\tau_{3D}\left(\frac{\varepsilon}{k_0 T}\right)^{1/2}, \tag{4}$$

where

$$\tau_{3D} = \tau_0\left(\frac{\varepsilon}{k_0 T}\right)^{r-1/2}, \tag{5}$$

is relaxation time in the bulk sample, τ_0 is independent of the electron energy constant, r is scattering parameter. The values of τ_0 and r for different scattering mechanisms are given in [16].

It is obvious that the differences in the power-law dependence of the relaxation time of the bulk sample - (r-1/2) and the superlattice - r, arise due to the different energy dependence of the density of quantum states.

It is known that at scattering of current carriers by acoustic phonons, point defects, and nonpolar optical phonons at high temperatures, the scattering parameter is the same, and is equal to $r = 0$. It is clear that under the action of the indicated scattering mechanisms, the longitudinal component of the relaxation time tensor does not depend on energy. Similar assumptions were made in [17] and a number of other works (see references in the same paper). The most convincing argument in favor of this statement is the results of [10], in which it was experimentally established that in SL *GaAs*/*AlAs* above the temperature 40K the relaxation time τ = const.

The nonequilibrium electron distribution function f is found in the approximation of the relaxation time from the Boltzmann kinetic equation

$$\vec{\upsilon}\frac{\partial f}{\partial\vec{r}} - e\vec{E}_0\frac{\partial f}{\hbar\partial\vec{k}} = -\frac{f_1}{\tau_{2D}}, \tag{6}$$

where $\vec{\upsilon}=\hbar^{-1}\partial\varepsilon(\vec{k})/\partial\vec{k}$ is electron velocity, $\vec{E_0}=-\partial\varphi/\partial\vec{r}$ is electric field intensity, φ is electric potential, $f_1=f-f_0$, $f_0=\left[1+\exp(\varepsilon-\varsigma)/k_0T\right]$ is the equilibrium Fermi-Dirac distribution function with a variable in space temperature T and chemical potential ζ, k_0 is the Boltzmann constant.

Solving (6) in the approximation of the relaxation time for the nonequilibrium addition to the distribution function we obtain

$$f_1=-\tau_{2D}\left(\frac{\partial f_0}{\partial\varepsilon}\right)\left[\frac{\varepsilon-\varsigma}{T}\vec{\upsilon}\cdot\nabla T-e\vec{\upsilon}\cdot\nabla\left(\varphi-\frac{\varsigma}{e}\right)\right], \tag{7}$$

The current density will be found from the ratio

$$\vec{j}=-\frac{2e}{(2\pi)^3}\int\vec{\upsilon}(\vec{k})\cdot f_1(\vec{k},\vec{r})d\vec{k}, \tag{8}$$

We assume that the vectors $\vec{E_0}$ and ∇T are directed along the SL axis which is compatible with the axis of the cylindrical coordinate system $0z$. Then, taking into account (7), for the current density we obtain

$$j=j_z=\sigma(\eta,\beta)\cdot\nabla_z\left(\frac{\varsigma}{e}-\varphi\right)-\alpha(\eta,\beta)\cdot\sigma(\eta,\beta)\nabla_zT \tag{9}$$

where α (η, β) and σ (η, β) are the Seebeck coefficient and electric conductivity along the SL axis.

The Seebeck coefficient will be found from relation [16]

$$\alpha(\eta,\beta)=\frac{\nabla_z\left(\frac{\varsigma}{e}-\phi\right)}{\nabla_zT}. \tag{10}$$

Assuming the current density in relation (9) equal to zero, for the Seebeck coefficient we obtain

$$\alpha(\eta,\beta)=-\frac{k_0}{e}\left[\frac{I_{1,2,0}(\eta,\beta)+\beta\, I_{0,2,2}(\eta,\beta)}{I_{0,2,0}(\eta,\beta)}-\eta\right]. \tag{11}$$

where

$$I_{k,l,m}(\eta,\beta)=\int_0^{\pi}F_k(\eta,z,\beta)\cdot(\sin z)^l\left(\sin\frac{z}{2}\right)^m dz, \tag{12}$$

$$F_k(\eta,z,\beta)=\int_0^{\infty}\frac{\exp\left(x-\eta+\beta\cdot\sin^2\frac{z}{2}\right)}{\left[1+\exp\left(x-\eta+\beta\cdot\sin^2\frac{z}{2}\right)\right]^2}x^k dx, \tag{13}$$

three-parameter Fermi integrals $\varepsilon_\perp=\hbar^2k_\perp^2/2m_\perp$, $x=\varepsilon_\perp/k_0T$ is reduced energy, $\eta=\zeta/k_0T$ is reduced chemical potential, $\beta=2\varepsilon_0/k_0T$ is reduced width of the conduction miniband in the direction of the superlattice axis, $z=ak_z$.

Figs. 2 and 3 show the results of the numerical analysis of the obtained relations

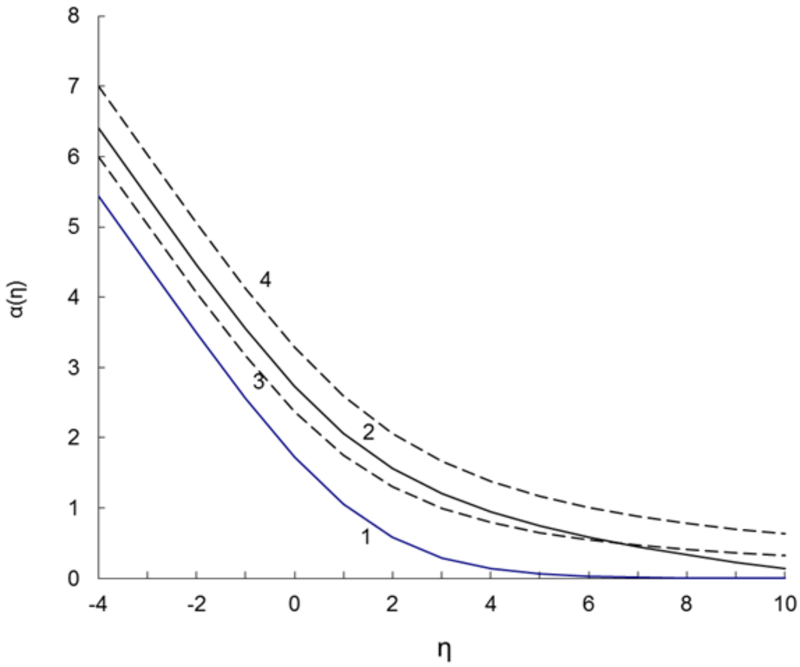

Fig. 2 Dependence of thermopower on the chemical potential at different values of the width of conduction miniband in the direction of the SL axis. 1 – at β = 1, 2 – at β = 10. Dashed curves correspond to the scattering of current carriers in a bulk material: by acoustic phonons - 3; by polar optical phonons - 4.

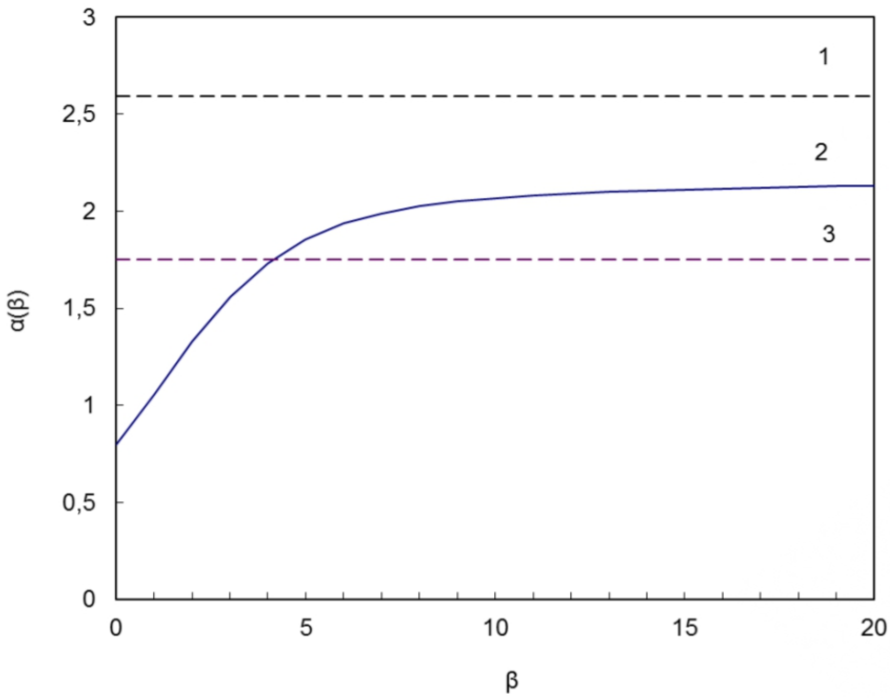

Fig. 3 Dependence of thermopower on the width of conduction miniband in the direction of the SL axis at η = 2. Dashed lines 1 and 3 correspond to the scattering of current carriers in a bulk material: 1 – by acoustic phonons; 3 – by polar optical phonons.

As follows from the analysis of relation (11), as the thickness of the superlattice layers decreases, the width of the conduction miniband in the direction k_z decreases, leading to a decrease in the Seebeck coefficient. If $\beta \to 0$, the value of the Seebeck coefficient asymptotically approaches the limit value

$$\alpha(\eta, 0) = -\frac{k_0}{e}\left[\frac{F_1(\eta)}{F_0(\eta)} - \eta\right], \tag{14}$$

and in the case of $\beta \to \infty$ to

$$\alpha(\eta, \infty) = -\frac{k_0}{e}\left[\frac{F_{5/2}(\eta)}{F_{3/2}(\eta)} - \eta\right], \tag{15}$$

where

$$F_k(\eta) = \int_0^\infty \frac{\exp(x-\eta)}{\left[1+\exp(x-\eta)\right]^2} x^k dx \quad , \tag{16}$$

one-parameter Fermi integrals of the *k-th* order [16].

An unlimited increase in β should be considered as an approximation of the width of the conduction miniband in the direction k_z to the width of the conduction band in the direction k . In this case, the movement of electrons along the SL axis approaches free one.

If $\eta < -4$, the electron gas of SL is nondegenerate, and (14) and (15) is converted to the form, respectively:

$$\alpha(\eta, 0) = -\frac{k_0}{e}[1-\eta]; \tag{17}$$

and

$$\alpha(\eta, \infty) = -\frac{k_0}{e}\left[\frac{5}{2} - \eta\right]. \tag{18}$$

For a bulk semiconductor whose composition is similar to the composition of the SL material at $\eta < -4$ relation (11) transforms into the well-known Pisarenko formula [16]

$$\alpha(\eta, \infty) = -\frac{k_0}{e}[2-\eta]\cdot \tag{19}$$

Conclusions

As a result of calculation by the numerical methods, Figs. 2 and 3 show the graphical dependences of the thermopower (in units - k_0/e) on the chemical potential and the width of the conduction miniband in the direction of the *0z* axis (in units k_0T) for SL and bulk material. The analysis shows that the degeneracy of the SL electron gas sets in the faster, the narrower the width of the conduction miniband in the direction of its axis. Obviously, this is due to a decrease in the total number of quantum states in the conduction band. Moreover, at $\beta << 5$ the SL thermopower is less than the thermopower of the bulk samples made of the same material. As the width of the conduction miniband increases, the SL thermopower grows, asymptotically approaching the limiting value at $\beta \geq 10$ in the bulk samples, which is quite obvious, since in this case the top of the conduction band in the direction of the *0z* axis ceases to play any role. It is clear that within the accepted assumptions, the thermopower does not depend on the period of the semiconductor

SL. This is explained by the form of the dispersion law and the nature of the energy dependence of the relaxation time.

Although a decrease in the width of the conduction miniband in the direction of the SL axis leads to a decrease in the thermopower, there are a number of factors that have a positive effect on its increase. For example, the electron-phonon entrainment, which in semiconductor superstructures at low temperatures can be of crucial importance [17]. In addition, a slight decrease in thermopower in comparison with bulk materials does not exclude an increase in the thermoelectric figure of merit of SL as a whole, due to a decrease in the lattice component of thermal conductivity caused by intense scattering of phonons at the boundaries of the layers.

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ТЕРМОЕРС В НАПІВПРОВІДНИКОВИХ НАДГРАТКАХ ПРИ РОЗСІЮВАННІ НОСІЇВ СТРУМУ НА ФОНОНАХ І ТОЧКОВИХ ДЕФЕКТАХ

В квазікласичному одномінізонному наближені досліджена термоЕРС напівпровідникових надграток (НГ) у випадку довільної статистики та при розсіюванні носіїв струму на акустичних фононах, точкових дефектах і неполярних оптичних фононах з урахуванням зміни часу релаксації в порівнянні з об'ємними матеріалами. Встановлена аналітична залежність термоЕРС від приведеної ширини зони провідності в напрямку осі надгратки. Показано, що термоЕРС надгратки збільшується із збільшенням ширини мінізони провідності, асимптотично наближаючись до граничного значення при $\beta \ge 10$. *Бібл. 17, рис. 3.*

Ключові слова: коефіцієнт термоЕРС, добротність надгратки, термоЕРС.

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ТЕРМОЭДС В ПОЛУПРОВОДНИКОВЫХ СВЕРХРЕШЕТКАХ ПРИ РАССЕЯНИЯ НОСИТЕЛЕЙ ТОКА НА ФОНОНАХ И ТОЧЕЧНЫХ ДЕФЕКТАХ

В квазиклассическом одноминизонном приближении исследована термоЭДС полупроводниковых сверхрешеток (СР) в случае произвольной статистики и при рассеянии носителей тока на акустических фононах, точечных дефектах и неполярных оптических фононах с учетом изменения времени релаксации по сравнению с объемными материалами. Установлена аналитическая зависимость термоЭДС от приведенной ширины зоны проводимости β *в направлении оси сверхрешетки. Показано, что термоЭДС сверхрешетки увеличивается с увеличением ширины минизоны проводимости, асимптотически приближаясь к предельному значению при* $\beta \ge 10$. *Библ. 17, рис.3.*

Ключевые слова: коэффициент термоЭДС, добротность сверхрешоток, термоЭДС.

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