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Thermoelectric Power Factor of Flat-Layer Semiconductor Structures

The influence of nanostructuring on the thermoelectric power factor of flat-layer semiconductor structures is studied in the quasi-classical one-miniband approximation. The change in the pulse relaxation time of current carriers in 2D structures as compared to their 3D counterparts in the case of mixed scattering of the pulse by acoustic phonons and point defects in the case of arbitrary statistics is taken into consideration. The analytical dependence of the thermoelectric power factor on the chemical potential and the width of the conduction miniband in the direction of the superlattice axis is established.

Keywords: 2D structures, quantum wells, conduction miniband, thermoelectric power factor, pulse relaxation time, electron thermal conductivity, thermoelectric figure of merit.

Formulation of the problem

A high-quality thermoelectric material should simultaneously have high thermoEMF and electrical conductivity and a low thermal conductivity. Since thermoEMF and electrical conductivity are determined exclusively by the electronic properties of material, they are often combined into thermoelectric power factor [1]

$$S = \alpha^2 \sigma , \tag{1}$$

where α and σ are coefficients of thermoEMF and electrical conductivity, respectively.

In order to increase power factor (hence, thermoelectric figure of merit), it is necessary to simultaneously increase coefficients of thermoEMF and electrical conductivity. However, an increase in the thermoEMF of material is accompanied by a decrease in its electrical conductivity, so maximizing of S value is a difficult task.

Analysis of recent studies and publications

In a number of works [2–5], the reduction of phonon thermal conductivity is considered as a promising method for increasing the figure of merit of nanostructured semiconductor

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materials. However, numerous experimental investigations devoted to the study of bulk thermoelectric materials with nanoscale inclusions and granular nanocomposites show that the thermoelectric properties of materials can be improved by increasing the thermoelectric power factor even without reducing the thermal conductivity of the lattice. In particular, it was shown in [6, 7] that in the superlattice of PbTe/PbTeSe quantum dots in the region of room temperatures, due to an increase in the thermoelectric power factor, a two-fold increase in the thermoelectric figure of merit was observed in comparison with the bulk PbTe sample. A similar pattern was also observed in nanogranular PbTe [8], Si and Ge [9].

The purpose of the work is to study the thermoelectric power factor of a flat-layer semiconductor structure in a quasi-classical one-miniband approximation with a mixed scattering of current carriers on acoustic phonons and point defects at arbitrary statistics and with regard to a change in relaxation time in 2D-structures as compared to their 3D counterparts.

Presentation of the main material. The presence of separation boundaries between the layers affects the electronic spectrum of superlattice (SL). While the movement of current carriers in the direction perpendicular to SL axis corresponds to the movement along a wide conduction zone, as in a bulk sample, the movement along the superlattice axis is limited by the nanostructuring layers. In this direction, the electronic spectrum has 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 the quasi-classical approximation $2\varepsilon_0 >> \hbar/\tau_{2D}$, eE_0 , $a\nabla_z k_0 T$ the law of electron dispersion in the lower SL miniband is described by the relation [10]

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

where $k_\perp = \left(k_x^2 + k_y^2\right)^{1/2}$, and k_z are the transverse and longitudinal components of the quasi-wave vector to the SL axis, $m_\perp^*$ is the transverse effective mass which is close in value to the effective mass of electrons of the semiconductor that forms the SL, a is the period of the SL, $2\varepsilon_0$ is the width of SL conduction miniband in the direction k_z , E_0 is the electric field strength, T is the average absolute temperature.

We will consider mixed scattering of electrons on acoustic phonons and point defects. To calculate the total relaxation time of the pulse of current carriers, we will use the Mathyssen rule

$$\frac{1}{\tau_{2D}} = \frac{1}{\tau_a} + \frac{1}{\tau_d}, \tag{3}$$

where τ_a and τ_d is pulse relaxation time on acoustic phonons and point defects in 2D structure.

With regard to the explicit form of τ_a and τ_d [11] and the change in the relaxation time of the pulse of current carriers in 2D structures as compared to bulk samples [12], the axial component of the tensor of pulse relaxation time of current carriers in in SL can be written as

$$\tau_{2D}(\varepsilon) = \tau_{0eff}\left(\frac{\varepsilon}{k_0 T}\right)^r, \tag{4}$$

where τ_{0a} and τ_{0d} are electron energy-independent constants, $\tau_{0eff} = \tau_{0a}\tau_{0d}\left(\tau_{0a}+\tau_{0d}\right)^{-1}$, r is scattering parameter.

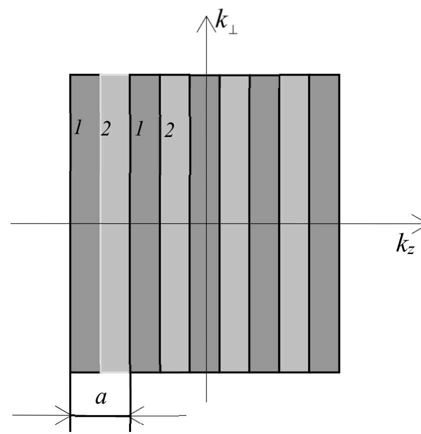

Fig. 1. Schematic of a flat-layer structure with quantum wells based on GaAs/AlAs. 1 – GaAs layer, 2 – AlAs layer

The electrical conductivity and thermoEMF will be found from the relations [4, 5]:

$$\sigma_{2D} = \frac{2e^2}{(2\pi)^3}\int \tau_{2D}(\varepsilon)\upsilon_z^2\left(-\frac{\partial f_0}{\partial \varepsilon}\right)\frac{\varepsilon}{k_0 T}d\vec{k}, \tag{5}$$

$$\alpha_{2D} = -\frac{k_0}{e}\left\{\frac{\int \tau_{2D}(\varepsilon)\upsilon_z^2\left(-\frac{\partial f_0}{\partial \varepsilon}\right)\frac{\varepsilon}{k_0 T}d\vec{k}}{\int \tau_{2D}(\varepsilon)\upsilon_z^2\left(-\frac{\partial f_0}{\partial \varepsilon}\right)d\vec{k}} - \frac{\varsigma}{k_0 T}\right\}, \tag{6}$$

where $f_0 = \left[1+\exp\left(\varepsilon-\varsigma\right)/k_0 T\right]^{-1}$ is the equilibrium Fermi-Dirac distribution function with spatially variable absolute temperature T and chemical potential ς, $\upsilon_z = \hbar^{-1}\,\partial\varepsilon\left(\vec{k}\right)/\partial k_z$ is the velocity of electrons in the direction of the superlattice axis, k_0 is the Boltzmann constant.

Taking into consideration (4) in formulae (5) and (6), we move from integration over the wave factor to integration over energy. In the spherical coordinate system for the coefficients of electrical conductivity and thermoEMF we obtain:

$$\sigma_{2D} = \sigma_0 I_{0,2,0}(\eta,\beta), \tag{7}$$

$$\alpha_{2D} = -\frac{k_0}{e}\left[\frac{I_{1,2,0}(\eta,\beta)+\beta\, I_{0,2,2}(\eta,\beta)}{I_{0,2,0}(\eta,\beta)} - \eta\right], \tag{8}$$

where

$$I_{k,l,m}(\eta,\beta) = \int_0^{\pi} F_k(\eta,z,\beta)(\sin z)^l \left(\sin\frac{z}{2}\right)^m dz, \tag{9}$$

$$F_k(\eta,z,\beta) = \int_0^{\infty} \frac{\exp\left(x-\eta+\beta\ \sin^2\frac{z}{2}\right)}{\left[1+\exp\left(x-\eta+\beta\ \sin^2\frac{z}{2}\right)\right]^2} x^k dx, \tag{10}$$

three-parameter integrals, σ_0 is a constant determined by the pulse dissipation mechanisms and material parameters of semiconductor, $\varepsilon_\perp = \hbar^2 k_\perp^2 / 2m_\perp^*$ is the energy component perpendicular to the superlattice axis, $x = \varepsilon_\perp / k_0 T$ is reduced energy, $\eta = \varsigma / k_0 T$ is reduced chemical potential, $z = ak_z$, $\beta = 2\varepsilon_0 / k_0 T$ is reduced width of the conduction miniband in the direction of the superlattice axis.

In the case of a bulk sample and a parabolic dispersion law $\beta = 0$, the three-parameter integrals (10) turn to one-parameter Fermi integrals [11]

$$F_k(\eta) = \int_0^{\infty} \frac{\exp(x-\eta)}{\left[1+\exp(x-\eta)\right]^2} x^k dx. \tag{11}$$

Calculation of thermoelectric power factor

As can be seen from relation (8) and Fig. 2, in 2D structures, as a result of a sharp change in the density of states near the Fermi level, and a change in the pulse relaxation time of current carriers as compared to bulk samples, an increase in the thermoEMF coefficient is observed. As long as thermoelectric power is proportional to the square of the thermoEMF coefficient, its increase is particularly relevant.

Thermoelectric power factor of superlattices depends on the chemical potential η and the width of conduction miniband, the dependence $S(\eta)$ having an extremum which shifts toward larger chemical potential values when the width of the conduction miniband increases.

Using the analytical dependences of the found kinetic coefficients, we find the ratio of thermoelectric powers of nanostructured and bulk samples.

$$n(\eta) = \frac{S_{2D}}{S_{3D}} = \left(\frac{\alpha_{2D}}{\alpha_{3D}}\right)^2 \left(\frac{\sigma_{2D}}{\sigma_{3D}}\right). \tag{12}$$

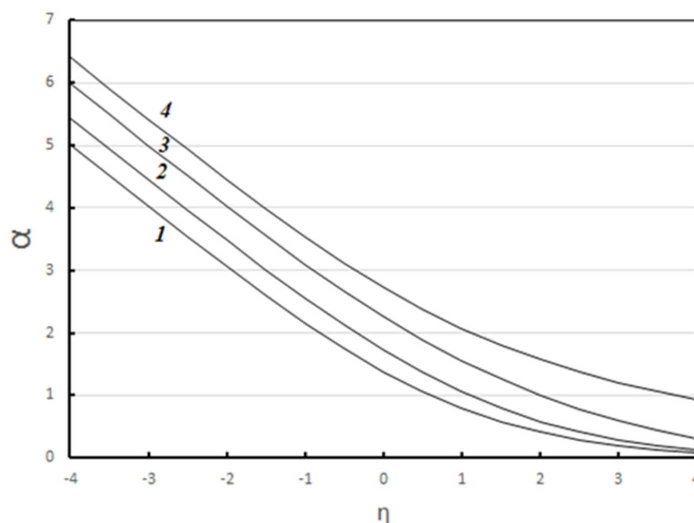

Fig. 2. Dependence of thermoEMF coefficient (in units k_0/e) on the reduced chemical potential: curve 1 for a bulk sample, curves 2–4 for the nanostructured 2D material. Curve 2 at β = 1, 3 – at β = 3, 4 – at β = 5

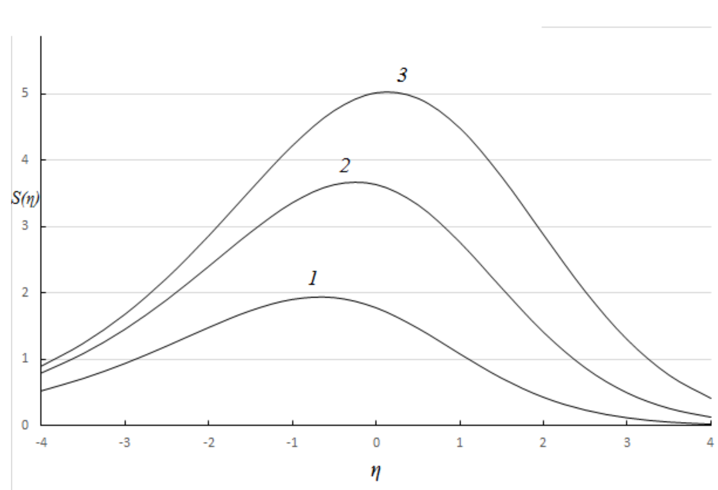

Fig. 3. Dependence of reduced thermoelectric power factor (in units $k_0\sigma_0/e$) on the reduced chemical potential: curve 1 for a bulk sample, curves 2, 3 for nanostructured material. Curve 2 for β = 3, 3 – for β = 5

Numerical analysis of (12) and Figs. 3 and 4, shows that thermoelectric power factor of nanostructured thermoelectrics is always greater than in the bulk samples, and increases with the increase in the width of the conduction miniband. In particular, in the region of room temperatures, under the condition of optimal doping, and with the width of conduction miniband $\beta = 1$, the power ratio is $n = 1.5$, with the width of $\beta = 3$ – $n = 2$, and with $\beta = 5$ it increases to $n = 2.5$. Therefore, it should be expected that nanostructuring will lead to an increase in the figure of merit of 2D samples, compared to their bulk counterparts, even without a decrease in phonon thermal conductivity.

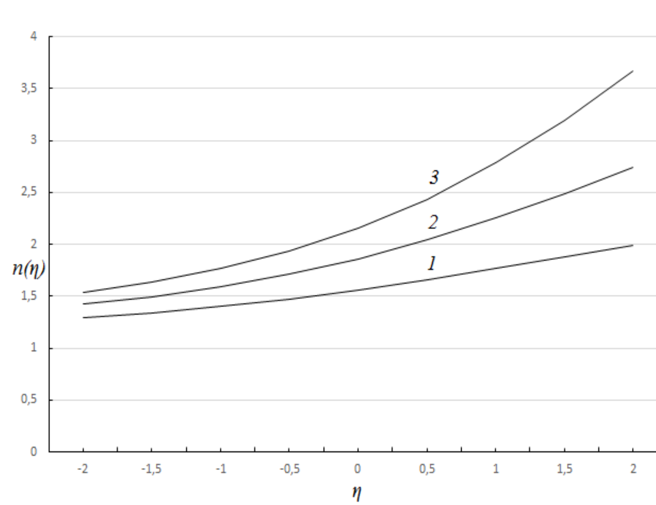

Fig. 4. Dependence of relative thermoelectric power on the reduced chemical potential: curve 1 for β = 1, 2 – for β = 3, 3 – for β = 5

Conclusions

An analytical expression was obtained that describes the effect of nanostructuring on the thermoelectric power of flat-layer semiconductor structures.

It is shown that thermoelectric power factor of the superlattices depends on the chemical potential η and the width of the conduction miniband, and the dependence $S(\eta)$ has a maximum that shifts toward larger chemical potential values when the width of the conduction miniband increases.

It was established that in 2D structures, compared to their 3D counterparts, due to a sharp change in the density of states near the Fermi level, and a change in the relaxation time of current carriers, an increase in the thermoelectric power factor is observed. This can contribute to an increase in the thermoelectric figure of merit even without reducing the phonon thermal conductivity.

Authors' information

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Тернопільський національний технічний університет імені Івана Пулюя, Україна

Коефіцієнт термоелектричної потужності плоскошарових напівпровідникових структур

В квазікласичному одномінізонному наближені досліджено вплив наноструктурування на коефіцієнт термоелектричної потужності плоскошарових напівпровідникових структур. Враховано зміну часу релаксації імпульсу носіїв струму в 2D структурах в порівнянні з їх 3D аналогами при змішаному розсіюванні імпульсу на акустичних фононах та точкових дефектах у випадку довільної статистики. Встановлено аналітичну залежність коефіцієнта термоелектричної потужності від хімпотенціалу та ширини мінізони провідності в напрямку осі надґратки.

Ключові слова: 2D структури, квантові ями, мінізона провідності, коефіцієнт термоелектричної потужності, час релаксації імпульсу, електронна теплопровідність, термоелектрична добротність.