THERMOEMF IN *Bi* NANOWIRES IN THE TRANSVERSE CONSTANT ELECTRIC FIELD

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• *This is a theoretical study of the thermoEMF in Bi quantum wires, when potential energy of carriers, for simplicity, is described by a paraboloid of revolution, and constant electric field is directed perpendicular to nanosystem axis. The thermoEMF is calculated with account of electron and hole scattering on the rough delta-correlated surface. In particular, it is shown that with increasing electric field intensity, the thermoEMF is of a non-monotonic nature and is mainly determined by electrons (the thermoEMF is negative).*

Introduction

In quantum wires, due to one-dimensionality of nanosystem under study, on the bottom of dimensionally quantized bands there appear peculiarities in the density of energy states. Exactly this factor brings about, in particular, the peculiarities of optical properties of nanowires [1 – 4], and has a pronounced effect, as will be shown below, on the kinetic coefficients in nanowires with a degenerate electron (hole) gas. This paper is a theoretical study of thermoEMF in quantum wires of *Bi* type in a model of quadratic potential. Such a model is frequently used in the calculations of the kinetic coefficients in nanowires [5, 6] and is theoretically justified [7]. If constant electric field *E* directed along the dimensional quantization axis of nanostructure, under certain conditions can have substantial impact on mobility [8], it is interesting to study the influence of *E* on thermoEMF in low-dimensional systems.

Formulation of the problem. General relationships

This paper studies the thermoEMF in *Bi* quantum wires with potential energy for carriers in the form of a paraboloid of revolution in constant electric field *E* directed perpendicular to axis of the investigated nanostructure. In the model under study the energy of electrons with the effective mass m_c in dimensionally quantized conduction band is of the form:

$$\varepsilon_c = \frac{\hbar^2 k_x^2}{2m_c} + \hbar\omega_c \left(n + k + 1\right) - \Delta_c , \ \Delta_c = \frac{e^2 E^2}{2m_c \omega_c^2} , \tag{1}$$

here k_x is wave vector of carrier along the nanowire axis, $\hbar\omega_c$ is dimensional quantization increment which is simply related to the value of potential energy ΔE_c at the boundary of nanostructure with radius *R*:

$$\hbar\omega_c = \frac{\hbar}{R}\sqrt{\frac{2\Delta E_c}{m_c}} .$$

As it immediately follows from (1), with increasing intensity of electrical field the bottom of dimensionally quantized band goes down to the energy gap. Exactly this circumstance leads to the fact that with account of electron scattering on the rough surface, the relaxation time depends on *E*, which results in a marked change of kinetic coefficients [8]. With growing *E,* carriers are "pressed" to nanostructure surface, i.e. their interaction with the rough surface is increased, which leads to reduction of relaxation time. In a similar manner one can calculate the energy of electrons with the

effective mass m_v in a dimensionally quantized valence band.

$$\varepsilon_v = \Delta - \frac{\hbar^2 k_x^2}{2m_v} - \hbar\omega_v \left(n + k + 1\right) + \Delta_v, \tag{2}$$

$$\Delta_v = \frac{e^2 E^2}{2m_v \omega_v^2}, \quad \hbar\omega_v = \frac{\hbar}{R}\sqrt{\frac{2\Delta E_v}{m_v}}.$$
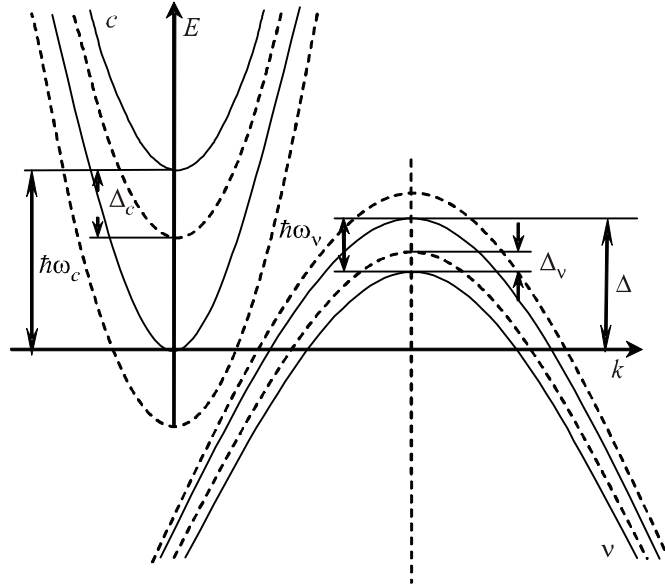

Fig. 1. Schematic of energy bands of Bi quantum wire in constant electric field.

Hereinafter for *Bi* nanowires we will consider the simplest model of overlapping bands (Fig. 1). Full lines in Fig. 1 show dimensionally quantized levels of *c* and *v* bands. Dashed lines represent carrier energies in constant electric field. Calculation of thermoEMF α_{xx} (weak pulling electrical field is directed along the *x* axis) was done with the use of general relationships relating α_{xx} to density of thermal energy flux γ_{xx} for carriers and to the electrical conductivity for electrons and holes [9]. In the approximation of relaxation time [10], the electrical conductivity and density of thermal energy flux for electrons take on the form:

$$\sigma_{xx}^{(c)} = \frac{\beta e^2 \hbar^2}{2V m_c^2} \sum_\alpha k_x^2 \tau_\alpha^{(c)} n_\alpha \left(1 - n_\alpha\right), \tag{3 a}$$

$$\gamma_{xx}^{(c)} = \frac{\beta e^2 \hbar^2}{2V m_c^2} \sum_\alpha \left(E_\alpha^c - \xi\right) k_x^2 \tau_\alpha^{(c)} n_\alpha \left(1 - n_\alpha\right), \tag{3 b}$$

here n_α is equilibrium function of carrier distribution with energy E_α^c, α is a set of quantum numbers describing electron state, $1 / \tau_\alpha^{(e)}$ determines full quantum-mechanical probability of particle scattering per unit time, ξ is chemical potential of system under study, $\beta = 1 / k_0 T$, *T* is temperature, *V* is volume of the main area of nanostructure.

Similarly one can write $\sigma_{xx}^{(h)}$, $\gamma_{xx}^{(h)}$ for holes in *v* band. Calculation of relaxation time τ_α will be done with regard to carrier scattering on the rough surface similarly to [8]. In the case of δ-like surface fluctuation it is not difficult to get:

$$\frac{1}{\tau_\alpha^{(c)}} = \frac{2m_c \omega_c^2 \gamma_0}{\hbar R^2 |k_x|} \left[n + k + 1 - N_c\right]^2, \tag{4}$$

$N_c = 2\Delta_c / \hbar\omega_c$, γ_0 describes fluctuation height. In the calculation of relaxation time for the case of

Gaussian fluctuation [11] at low temperatures (exactly at low temperatures carrier scattering on the rough surface is most active), $1/\tau_\alpha^{(e)}$ is described by relationship (4) where γ_0 should be replaced by $\pi\Delta_0^2\Lambda^2$ (Δ_0 is the height of Gaussian fluctuation, Λ is its length). Note that $\tau_\alpha^{(e)}$ (for any fluctuation type) is precisely transport relaxation time used when solving the Boltzmann kinetic equation. $\tau_\alpha^{(h)}$ for holes is written similarly. As a result, the expression for thermoEMF after summation over k_x takes on the form:

$$\alpha_{xx} = -\frac{k_0}{e}\left\{\sum_{n,m}\left[\nu\frac{F_2(\eta_{nm}^c) - \eta_{nm}^c F_1(\eta_{nm}^c)}{(n+m+1+N_c)^2} - \frac{F_2(\eta_{nm}^v) - \eta_{nm}^v F_1(\eta_{nm}^v)}{b(n+m+1+aN_c)^2}\right]\right\}\times$$
$$\times\left\{\sum_{n,m}\left[\nu\frac{F_1(\eta_{nm}^c)}{(n+m+1+N_c)^2} + \frac{F_1(\eta_{nm}^v)}{b(n+m+1+aN_c)^2}\right]\right\}^{-1}, \tag{5}$$

$$a = \left(\frac{m_h}{m_c}\right)^{\frac{1}{2}}\left(\frac{\Delta E_c}{\Delta E_h}\right)^{\frac{3}{2}}, \quad b = \frac{\Delta E_h}{\Delta E_c},$$

$$\eta_{nm}^c = \beta\left[\Delta_c + \xi - \hbar\omega_c(n+m+1)\right],$$

$$\eta_{nm}^v = \beta\left[\Delta + \Delta_v - \xi - \hbar\omega_v(n+m+1)\right],$$

$$F_k(\eta) = \int_0^\infty dx \cdot x^k \cdot \frac{e^{x-\eta}}{(e^{x-\eta}+1)^2}, \quad F_1(\eta) = \ln(e^\eta + 1),$$

ν is the number of conduction bands taking part in kinetic processes. Chemical potential ξ is found from condition of electric neutrality of the investigated nanostructure (the number of electrons in dimensionally quantized c bands is equal to the number of holes in v band):

$$\nu\sqrt{\frac{m_c}{m_v}}\sum_{n,m}F_{1/2}(\eta_{nm}^c) = \sum_{n,m}F_{1/2}(\eta_{nm}^v). \tag{6}$$

An analytical solution of equation (6) for chemical potential can be found for partial cases.

If carriers are on the lowest dimensionally quantized level ($n = m = 0$), the electron and hole gas is degenerate (chemical potential is positive and $\beta\xi \gg 1$), then at $m_c \ll m_v$ from (6) it is not difficult to determine ξ:

$$\xi - \hbar\omega_c = \Delta + \Delta_v - (\hbar\omega_c + \hbar\omega_v), \quad \left(\frac{\Delta_v}{\Delta_c} = \frac{\Delta E_c}{\Delta E_v} > 1\right).$$

$(\xi - \hbar\omega_c)$ is chemical potential counted from the bottom of dimensionally quantized band.

In such a simple model the thermoEMF assumes the form:

$$\alpha_{xx} = -\frac{k_0}{e}\frac{\pi^3}{3}\frac{1 - \frac{1}{b\nu}\left(\frac{1+N_c}{1+aN_c}\right)^2}{\Delta + \Delta_v - (\hbar\omega_c + \hbar\omega_v)}. \tag{7}$$

Hence, the thermoEMF is negative, i.e. it is determined by electrons and is reduced with growing the electric field intensity E.

In the opposite case of the nondegenerate electron and hole gases (it is valid for small quantum wire radii $d \ll 500$ Å, at $T = 77$ K [3]), as it follows from equation (6), chemical potential is found from the relation:

$$\nu\sqrt{\frac{m_c}{m_v}}e^{\eta_{00}^c} = e^{\eta_{00}^v}. \tag{8}$$

As a result

$$\alpha_{xx}^{(nd)} = -\frac{k_0}{e}\left\{2 + \beta\left[\frac{1}{2}\ln(\nu^2\frac{m_c}{m_h}) + \left(\hbar\omega_c + \hbar\omega_v - \Delta + \Delta_v + \Delta_c\right)\right]\right\}. \tag{9}$$

In the general case the thermoEMF was calculated by the ratio (5) with regard to dimensionally quantized v and c bands with typical values of quantum wire parameters: $\Delta E_c = 0.5$ eV, $\Delta E_v = 0.3$ eV, $\Delta = 0.038$ eV, $m_c = 0.01\ m_0$, $m_v = 0.1\ m_0$, at $R = 500$ Å. The thermoEMF as a function of constant electric field intensity is given in Fig. 2.
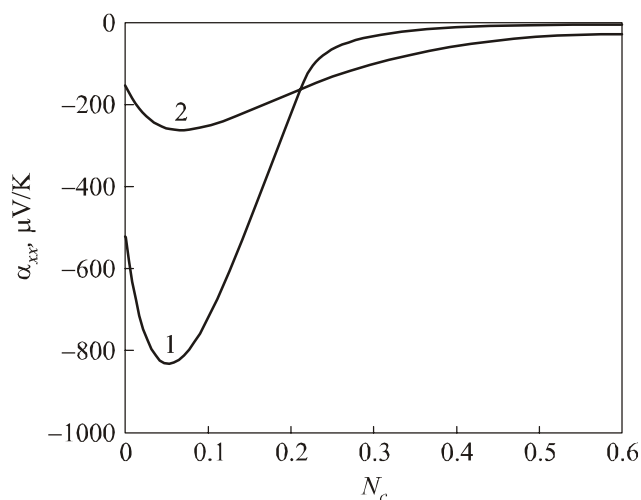

Fig. 2. Specific thermoEMF of quantum wire as a function of transverse electric field intensity.

The dependence 1 was obtained at $T = 10$ K, the dependence 2 was calculated at $T = 50$ K. As it immediately follows from Fig. 2, with increasing temperature the absolute value of thermoEMF is reduced and with increasing E it tends to zero, while remaining negative.

In the nanowires, as a consequence of nanostructure single-dimensionality, peculiarities arise in the density of states on the bottom of each dimensionally quantized zone. Therefore, with growth of constant electric field intensity, the extremes, for instance, of dimensionally quantized v bands, rising in the energy, can cross chemical potential, which, naturally, leads to peculiarities of kinetic coefficients (for instance, mobility). However, in thermoEMF these peculiarities are not very vivid since α_{xx} is determined by the ratio of thermal energy carriers flux to the electrical conductivity.

At $E = 0$, the holes contribute considerably to thermoEMF, reducing its absolute value. With increasing the electric field intensity (for the above considered nanowire parameters $a \sim 7$), the contribution of holes to thermoEMF is quickly reduced, as a result of which a characteristic minimum appears on the dependence of α_{xx} on N_c (Fig. 2).

Discussion of the results. Conclusion

Consequently, the external electric field gives a unique opportunity to control the value of thermoEMF which holds out a hope of the instrumental use of the predicted effect. Note, in conclusion, that strong anisotropy of effective masses in *Bi* nanowires (depending on the direction of crystallographic axes, masses for electrons in *c*-band change from $0.001\ m_0$ to $0.26\ m_0$, in the valence band from $0.059\ m_0$ to $0.634\ m_0$ [4]) has influence on the magnitude of effect under consideration,

which preserves dependence of thermoEMF on almost unvaried.

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Submitted 18.05.2011.