JOURNAL OF NANO- AND ELECTRONIC PHYSICS
Vol. 9 No 2, 02024(4pp) (2017)

ЖУРНАЛ НАНО- ТА ЕЛЕКТРОННОЇ ФІЗИКИ
Том 9 № 2, 02024(4cc) (2017)

The Kinetic Effects, Caused by Thickness Fluctuations of Quantum Semiconductor Wire

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(Revised 19.03.2017, revised manuscript received 26 April 2017; published online 28 April 2017)

The electrical conductivity, thermopower and thermal conductivity of semiconductor quantum wire conditioned by a random field of Gaussian fluctuations of wire thickness are theoretically determined. We present the results for cases nondegenerate and generate statistics of carriers. The considered mechanism of relaxation of the carriers is essential for sufficiently thin and clean wire from the A3B5 and A4B6 type of semiconductors at low temperatures. The quantum size effects that are typical of quasi-one-dimensional systems were revealed.

Keywords: Semiconductor quantum wire, Gaussian fluctuations of thickness, Electrical conductivity, Thermopower, Thermal conductivity.

DOI: 10.21272/jnep.9(2).02024

PACS numbers: 73.21.Fg, 73.50.Lw

1. INTRODUCTION

In thin semiconductor wire quantization of electron energy spectrum leads to quantum size effects, which are found in the kinetic parameters of quasi-onedimensional system, which are also depended on the mechanism of carriers scattering. In modern nanoelectronics technologies the influence of random field associated with fluctuations in the thickness of semiconductor quantum wires, generally speaking, cannot be ignore [1]. The aim of this work is to generalize and refine previous studies [2] the proliferation impact of such fluctuations on the basic kinetic characteristics of semiconductor quantum wire.

2. THEORETICAL MODEL

In [4] the model of semiconductor quantum wires with cross sizes, limited by thickness d (in the direction of coordinate axis z) by one-dimensional a potential pit $V(z)$ with infinitely high walls and for the width (towards y) parabolic potential βy^2 $(\beta > 0)$ are considered. The constant magnetic field $\mathbf{H}$ is directed along the wire (axis x); components of the vector potential of magnetic field: $A_x = A_y = 0$, $A_z = H_y$.

In the mean field theory (one-electron approximations) [5] Hamiltonian system has the form

$$\hat{H} = -\frac{\hbar^2}{2m_\perp}\Delta_\perp + \frac{1}{2m_z}\left(-i\hbar\frac{\partial}{\partial z} + \frac{e}{c}A_z\right)^2 + V(z) + \\ +\beta y^2 + U(\mathbf{r}_\perp), \qquad (1)$$

where $\Delta_\perp = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$, $m_\perp = m_x = m_y = m$ i m_z – effective mass of the electron along appropriate directions, e - the absolute value of the electron charge,

$$V(z) = \begin{cases} 0, -d/2 \le z \le d/2, \\ \infty, z < -d/2, z > d/2, \end{cases} \qquad (2)$$

$$U(\mathbf{r}_\perp) = \alpha[\xi_1(\mathbf{r}_\perp) - \xi_2(\mathbf{r}_\perp)] \qquad (3)$$

– potential energy of an electron in a random field, caused by fluctuations in the thickness of the wire, $\alpha = \partial E_c / \partial d$, E_c – the bottom of the conduction band, $\xi_{1,2}(\mathbf{r}_\perp)$ – a random functions that determine the amplitude of fluctuations on different surfaces of the wire perpendicular to the axis z. Interaction (3) of carriers with a random field is considered a disturbance which causes the quantum transitions in the translational movement along the wire (in the direction of the axis x). We confined by contribution of lower quantum size energy levels of the electron cross motions. In approximation of account of electron states with a certain parity in the z-axis wave function of unperturbed problem is

$$\psi_{k_x}(\mathbf{r}) = \sqrt{\frac{2}{\pi^{1/2}Ldy_0}}\exp\left(ik_x x - \frac{y^2}{2y_0^2}\right)\cos\left(\frac{\pi}{d}z\right), \qquad (4)$$

where L – wire length ($L >> d$),

$$y_0 = \hbar^{1/2}\left[2m\left(\beta + \frac{e^2H^2}{2m_z c^2}\right)\right]^{-1/4}. \qquad (5)$$

The energy of an electron in a state (4):

$$E(k_x) = \frac{\hbar^2 k_x{}^2}{2m} + \frac{\pi^2\hbar^2}{2m_z d^2} + \hbar\left[\frac{1}{2m}\left(\beta + \frac{e^2H^2}{2m_z c^2}\right)\right]^{1/2}. \qquad (6)$$

3. THE RELAXATION TIME

The inverse relaxation time of the electron along the wire length at the scattering of fluctuation field (3) has the form

$$\frac{1}{\tau_n(k_x)} = \frac{2\pi}{\hbar}\sum_{k'_x}\left\langle\left\langle\left|\left\langle k'_x\right|U\left|k_x\right\rangle\right|^2\right\rangle\right\rangle\left(1 - \frac{k'_x}{k_x}\right)\times \\ \times\delta\left[E(k_x) - E(k'_x)\right], \qquad (7)$$

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where double brackets $\langle\langle ... \rangle\rangle$ determine averaging over the random field. Fluctuations on different surfaces of wire are considered independent and on one surface - Gauss fluctuations:

$$\left\langle\left\langle \xi_i(\mathbf{r}_{\perp 1})\xi_j(\mathbf{r}_{\perp 2})\right\rangle\right\rangle = \delta_{ij}\Delta_i^2 \exp\left[-\frac{(\mathbf{r}_{\perp 1}-\mathbf{r}_{\perp 2})^2}{2\Lambda_i^2}\right], \qquad (8)$$
$$\left\langle\left\langle \xi_i(\mathbf{r}_{\perp})\right\rangle\right\rangle = 0,\, i,j = 1,2\,.$$

After calculating (7) with (3) and (8) we find a general expression for the relaxation time [2]

$$\frac{1}{\tau_n(k_x)} = \frac{\alpha^2 m\sqrt{2\pi}}{\hbar^3 |k_x|}\sum_{i=1}^{2}\frac{(\Delta_i\Lambda_i)^2}{\sqrt{y_0^2+\Lambda_i^2}}\exp(-2\Lambda_i^2 k_x^2)\,. \qquad (9)$$

4. STATIC CONDUCTIVITY

For electronic conductivity from the kinetic Boltzmann equation in the relaxation time approximation, we get next:

$$\sigma_n = \frac{2\hbar^2 e^2}{m^2}\int_0^\infty\left(-\frac{\partial f_0}{\partial\varepsilon}\right)k_x^2\tau_n(|k_x|)\,dk_x\,, \qquad (10)$$

where $f_0 = \{\exp[(\varepsilon-\mu)/k_BT]+1\}^{-1}$ – distribution function of the Fermi-Dirac, $\varepsilon = \hbar^2 k_x^2/2m$, μ – chemical potential, measured from the quantum-dimensional level of movement of electrons across the wire, $2\sum_{k_x} f_0(k_x) = N$ – the total number of electrons in a wire.

In [2], taking into account the general expression for the relaxation time (9), a bit bulky final expressions for conductivity σ_n, found from (10) were obtained and analyzed for arbitrary values of Δ_i, Λ_i, magnetic field H and temperature T.

Dependencies of on on longitudinal magnetic field H are associated with compression of wave function of electrons across the wire (along the axis y) and are determined by factor $\left[y_0^2(H)+\Lambda_i^2\right]^{-1/2}$ (See. (5)). At $y_0^2(H) >> \Lambda_i^2$ and extremely strong magnetic field $e^2H^2/2m_zc^2 >> \beta$, this leads to the appearance in σn the factor $H^{-1/2}$.

For simplicity in (9) the case $H = 0$ $\Lambda_1 = \Lambda_2 = \Lambda$ was considered. Then for relaxation time $\tau_n(\varepsilon)$ of an electron with energy ε, we have:

$$\tau_n(\varepsilon) = B\varepsilon^{1/2}\exp(\gamma\varepsilon)\,, \qquad (11)$$

where

$$B = \hbar^2\Big/\left[\alpha^2(\pi m)^{1/2}(A_1+A_2)\right], \qquad (12)$$

$$A_i = \frac{(\Delta_i\,\Lambda)^2}{\sqrt{y_0^2+\Lambda^2}}\,,\ \gamma = \frac{4m\Lambda^2}{\hbar^2}\,. \qquad (13)$$

According to (10) σ_n conductivity can be written in the form [3]:

$$\sigma_n = e^2\mathbf{K}_0\,, \qquad (14)$$

where

$$\mathbf{K}_0 = \frac{2^{3/2}}{\pi\hbar m^{1/2}}\int_0^\infty \tau_n(\varepsilon)\left(-\frac{\partial f_0}{\partial\varepsilon}\right)\varepsilon^{1/2}d\varepsilon\,. \qquad (15)$$

For nondegenerate case of semiconductor wire including (11) – (13) we obtain:

$$\sigma_n = \frac{2\hbar^2 e^2 n}{\pi\alpha^2 m^{3/2}}\frac{(k_BT)^{1/2}}{(1-\gamma k_BT)^2}(A_1+A_2)^{-1}\,, \qquad (16)$$

where $n = N/L$ – the number of electrons per unit length. Equation (16) fair when $1-\gamma k_BT > 0$ and $\hbar^2(1-\gamma k_BT)\pi^2/2mk_BTl^2 >> 1$, where l – is the lattice constant along the axis of the wire. The first condition associated with that the relaxation time ((9), (11) – (13) inreases exponentially with the energy of the electron, and Maxwell distribution decreases exponentially. Therefore, for the efficiency of scattering by Gauss fluctuations is significantly that the de Broglie "heat" wavelength of the charge carrier exceeded the value of the correlation radius Λ.

The second condition is associated with a choice of infinite upper limit of the integral (10), (15) and is usually performed. In the case of low temperatures and $\gamma k_BT << 1$ the electron mobility along the axis of the wire is $u_n \propto (k_BT)^{1/2}$ which for the temperature dependence resembles a dipole scattering [4] for three-dimensional semiconductor materials.

For degenerate case and $k_BT << \mu$ conductivity along the axis of wire including the general expression for the relaxation time (9) is

$$\sigma_n \approx \frac{4e^2\hbar}{\alpha^2 m\sqrt{2\pi}}\mu\times$$
$$\times\left[A_1\exp(-2k_F^2\Lambda_1^2)+A_2\exp(-2k_F^2\Lambda_2^2)\right]^{-1}, \qquad (17)$$

where $k_F^2 = (2m/\hbar^2)\mu$. Temperature dependence σ_n is determined of chemical potential of one-dimensional electron gas

$$\mu \approx \mu_0\left[1+\frac{\pi^2}{12}\left(\frac{k_BT}{\mu_0}\right)^2\right], \qquad (18)$$

$$\mu_0 = \frac{\hbar^2}{8m}(\pi n)^2\,. \qquad (19)$$

According to calculations for wires A3B5 materials (eg, GaAs [2]) and A4B6 mechanism of relaxation of charge carriers at random roughness of boundaries is essential at low temperatures $k_BT < \hbar^2/4m\Lambda^2$ for clean enough samples and nanometer thicknesses.

The effects of localization type [5], which arising in quasi-one-dimensional systems in heavy clutter (or at very high concentrations of impurities) which can not be explained within the theory of weak scattering in our work are not considered. So we obtained temperature dependence of conductivity significantly different from the consequences of the theory of localization [5].

5. THERMOPOWER

According to kinetic Boltzmann equation thermoelectric power Sxx can be written [3, 6] in view

$$S_{xx} = -\frac{1}{eT}\mathbf{K}_0^{-1}\mathbf{K}_1 , \qquad (20)$$

where K_0 is determined by formula (15),

$$\mathbf{K}_1 = \frac{2^{3/2}}{\pi\hbar m^{1/2}}\int_0^\infty \tau_n(\varepsilon)\left(-\frac{\partial f_0}{\partial\varepsilon}\right)(\varepsilon-\mu)\varepsilon^{1/2}d\varepsilon . \qquad (21)$$

After the reshuffle in the (20) formulas (15) and (21) with (11) we obtain [4] at $\gamma k_BT < 1$:

$$S_{xx} = -\frac{1}{eT}\left(\frac{F_{2\gamma}}{F_{1\gamma}} - \mu\right), \qquad (22)$$

where

$$F_{2\gamma} = \int_0^\infty \varepsilon^2\left(-\frac{\partial f_0}{\partial\varepsilon}\right)e^{\gamma\varepsilon}d\varepsilon ,\ F_{1\gamma} = \int_0^\infty \varepsilon\left(-\frac{\partial f_0}{\partial\varepsilon}\right)e^{\gamma\varepsilon}d\varepsilon . \qquad (23)$$

For nondegenerate statistics of carriers $f_0 = \exp\left[(\varepsilon-\mu)/k_BT\right]$ from (22) and (23) we find at $1 - \gamma k_BT > 0$

$$S_{xx} = -\frac{k_B}{e}\left(\frac{2}{1-\gamma k_BT} - \frac{\mu}{k_BT}\right), \qquad (24)$$

where the chemical potential of one-dimensional electron gas

$$\mu = k_BT\ln\left[\hbar n\left(\frac{\pi}{2mk_BT}\right)^{1/2}\right]. \qquad (25)$$

Due to summand $2(1 - \gamma k_BT) - 1$ there is the possibility of increasing thermoelectric power for one-dimensional quantum wire.

For the case of highly degenerate one-dimensional electron gas at $k_BT << \mu$, using the standard for this limiting case approach [5], we get

$$S_{xx} = -\frac{\pi^2}{3e}k_B\left(\frac{k_BT}{\mu}\right)(1+\gamma\mu), \qquad (26)$$

where the chemical potential $\mu(T)$ determined by question (18), (19). Due to summand $\gamma\mu$ in (26) we have a theoretical possibility to increase the value of thermoelectric power for considered one-dimensional case.

6. THERMOPOWER

According to [3, 6] coefficient of thermal conductivity is determined by the formula:

$$\varkappa_n = \frac{1}{T}\left(\mathbf{K}_2 - \frac{\mathbf{K}_1^2}{\mathbf{K}_0}\right), \qquad (27)$$

where

$$\mathbf{K}_2 = \frac{2^{3/2}}{\pi\hbar m^{1/2}}\int_0^\infty \tau_n(\varepsilon)\left(-\frac{\partial f_0}{\partial\varepsilon}\right)(\varepsilon-\mu)^2\varepsilon^{1/2}d\varepsilon . \qquad (28)$$

For nondegenerate system of charge carriers for $1 - \gamma k_BT > 0$ we have:

$$\mathbf{K}_0 = \frac{2\hbar^2 n}{\pi\alpha^2 m^{3/2}}\frac{(k_BT)^{1/2}}{(1-\gamma k_BT)^2}(A_1+A_2)^{-1} , \qquad (29)$$

$$\mathbf{K}_1 = \left(\frac{F_{2\gamma}}{F_{1\gamma}} - \mu\right)\mathbf{K}_0 , \qquad (30)$$

$F_{2\gamma}$ and $F_{1\gamma}$ we find from (23).

$$\mathbf{K}_2 = \frac{2\hbar^2 n}{\pi m^{3/2}\alpha^2}\frac{(k_BT)^{1/2}}{(1-\gamma k_BT)^2}\times \\ \times\left[\frac{6(k_BT)^2}{(1-\gamma k_BT)^2} - \frac{4\mu k_BT}{(1-\gamma k_BT)} + \mu^2\right](A_1+A_2)^{-1} . \qquad (31)$$

According to formulas (29) – (31) and (27) we obtain the final result for the thermal conductivity of semiconductor quantum wire caused by fluctuations in the thickness:

$$\varkappa_n = \frac{1}{T}\left\{\frac{2\hbar^2 n}{\pi\alpha^2 m^{3/2}}\frac{(k_BT)^{1/2}}{(1-\gamma k_BT)^2}\times \right. \\ \left. \times\left[\frac{2(k_BT)^2}{(1-\gamma k_BT)^2} - \frac{2\mu k_BT}{(1-\gamma k_BT)} + \frac{3}{4}\mu^2\right](A_1+A_2)^{-1}\right\}, \qquad (32)$$

where μ – chemical potential one-dimensional electron gas (see. (25)).

Using (16) and (32), we find the relation

$$\frac{\varkappa_n}{\sigma_n T} = 2\left(\frac{k_B}{e}\right)^2\times \\ \times\left[\frac{1}{(1-\gamma k_BT)^2} - \frac{\mu}{k_BT}\frac{1}{(1-\gamma k_BT)} + \frac{3}{8}\left(\frac{\mu}{k_BT}\right)^2\right], \qquad (33)$$

which shows that Wiedemann-Franz law holds only at $\gamma k_BT << 1$ and $\mu << k_BT$.

For case of strongly degenerate electron gas at $k_BT << \mu$ and $\Lambda_1 = \Lambda_2 = \Lambda$ we have:

$$\mathbf{K}_0 = \frac{2^{3/2}\mu\hbar}{\alpha^2 m\pi^{1/2}}(A_1+A_2)^{-1}e^{\gamma\mu} ,\ \sigma_n = e^2\mathbf{K}_0 , \qquad (34)$$

$$\mathbf{K}_1 = \frac{\pi^2}{3}\frac{(k_BT)^2}{\mu}(1+\gamma\mu)\mathbf{K}_0 , \qquad (35)$$

$$\mathbf{K}_2 = \frac{2^{3/2}\pi^{1/2}}{3}\frac{\hbar\mu(k_BT)^2}{\alpha^2 m}(A_1+A_2)^{-1}e^{\gamma\mu} . \qquad (36)$$

From (27) and (34) – (36) obtain

$$\varkappa_n = \frac{2^{2/3}\pi^{1/2}}{3T}\frac{\mu\hbar}{m\alpha^2}\left(k_B T\right)^2\left(A_1 + A_2\right)^{-1} e^{\gamma\mu} \times \\ \times\left[1 - \frac{\pi^3}{3}\left(\frac{k_B T}{\mu}\right)^2 (1+\gamma\mu)^2\right]. \qquad (37)$$

Relation

$$\frac{\varkappa_n}{\sigma_n T} = \frac{\pi}{3}\left(\frac{k_B}{e}\right)^2\left[1 - \frac{\pi^3}{3}\left(\frac{k_B T}{\mu}\right)^2\left(1+\gamma\mu\right)^2\right]. \qquad (38)$$

characterizes the accuracy with which performed Wiedemann-Franz law to degenerate semiconductor quantum wire.

7. SUMMARY

Based on the expressions of the relaxation time of charge carriers, conductivity, thermoelectric power and thermal conductivity of quantum semiconductor wire it is shown that the mechanism of relaxation is caused by a random field Gauss fluctuations in the thickness of wire may be effective for sufficiently thin and clean wire from the material A3B5 and A4B6 in thicknesses of nanometric size. The possibility of increasing some kinetic parameters of quasi-one-dimensional systems is revealed.

Кинетические эффекты, обусловленные флуктуациями толщины квантовой полупроводниковой проволоки

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Теоретически определены электропроводность, термоэдс и теплопроводность квантовой полупроводниковой проволоки вследствие гауссовськиx флуктуаций толщины проволоки. Результаты приведены для случаев невырожденной и вырожденной статистики носителей заряда. Рассмотрен механизм релаксации носителей заряда является существенным для достаточно тонкого и чистого проволоки из полупроводников типа A3B5 и A4B6 при низких температурах. Определены квантово-размерные эффекты, характерные для квазиодномерных систем.

Ключевые слова: Квантовая полупроводниковая проволока, Гауссовские флуктуации толщины, Электропроводность, ТермоЭДС, Теплопроводность.

Кінетичні ефекти, обумовлені флуктуаціями товщини квантового напівпровідникового дроту

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Теоретично визначено електропровідність, термоерс і теплопровідність квантового напівпровідникового дроту внаслідок гаусівських флуктуацій товщини дроту. Результати наведено для випадків невиродженої і виродженої статистики носіїв заряду. Розглянутий механізм релаксації носіїв заряду є суттєвим для достатньо тонкого і чистого дроту з напівпровідників типу A_3B_5 і A_4B_6 при низьких температурах. Визначено квантово-розмірні ефекти, характерні для квазіодновимірних систем.

Ключові слова: Квантовий напівпровідниковий дріт, Гауссові флуктуації товщини, Електропровідність, ТермоЕРС, Теплопровідність.

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