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## СТРОЕНИЕ И СВОЙСТВА НАНОРАЗМЕРНЫХ И МЕЗОСКОПИЧЕСКИХ МАТЕРИАЛОВ

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# Phonon Drag Thermopower in Quantum Wire with Parabolic Confinement Potential

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The quantitative theory of phonon drag thermopower for the one-dimensional electron gas in a quantum wire with a parabolic confinement potential is developed. The temperature gradient is directed along the axis of a quantum wire. As assumed, the Fermi level is located between the zero and first levels of a size quantization. Using the Boltzmann kinetic equation, the phonon and electronic parts of a thermoelectric power are calculated. For comparison, numerical calculations of the temperature and concentration dependences of the phonon and diffusion parts of a thermoelectric power are carried out. As shown, the phonon drag makes a main contribution in thermopower within the temperature interval 2–20 K.

**Key words:** quantum wire, phonon drag, parabolic potential, energy spectrum, thermoelectric effects, diffusion thermopower, phonon thermopower.

Розроблено кількісну теорію термоерс фононного перетягання для одновимірного електронного газу в квантовому дроті з параболічним обмежувальним потенціялом. Ґрадієнт температури спрямовано уздовж осі квантового дроту. Передбачається, що рівень Фермі розташований між нульовим і першим рівнями розмірного квантування. З використанням Больц-

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маннового кінетичного рівняння обчислено фононну й електронну частини термоерс. Для порівняння було проведено чисельні розрахунки температурної та концентраційної залежностей фононної й дифузійної частин термоерс. Показано, що фононне перетягання дає основний внесок у термоерс в інтервалі температур 2–20 К.

**Ключові слова:** квантовий дріт, фононне перетягання, параболічний потенціял, енергетичний спектер, термоелектричні ефекти, термодинаміка дифузії, теплова енергія фононів.

Разработана количественная теория термоэдс фононного увлечения для одномерного электронного газа в квантовой проволоке с параболическим ограничивающим потенциалом. Градиент температуры направлен вдоль оси квантовой проволоки. Предполагается, что уровень Ферми расположен между нулевым и первым уровнями размерного квантования. С использованием кинетического уравнения Больцмана вычислены фононная и электронная части термоэдс. Для сравнения были проведены численные расчёты температурной и концентрационной зависимостей фононной и диффузионной частей термоэдс. Показано, что фононное увлечение вносит основной вклад в термоэдс в интервале температур 2–20 К.

**Ключевые слова:** квантовая проволока, фононное увлечение, параболический потенциал, энергетический спектр, термоэлектрические эффекты, термодинамика диффузии, тепловая энергия фононов.

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## 1. INTRODUCTION

In recent years, a significant number of papers were devoted to experimental and theoretical investigations of thermopower in low-dimensional systems have appeared [1–3]. The limited motion of electrons in such systems leads to the fact that the kinetic phenomena in them sharply differ from the electronic transport phenomena in bulk samples.

Quantum-size structures produced in recent decades have attracted attention also because of possibility of their using in thermoelements with high thermoelectric efficiency. Studies in this field have shown that it is possible to increase the thermoelectric efficiency two or three times by preparing thermoelectric structures with quantum wells [4].

In this paper, we discuss the temperature dependence of the thermoelectric power of a degenerate electron gas in a quantum wire with a parabolic confinement potential in the low-temperature range of 1–20 K, where the phonon drag effect plays an important role. Due to confinement, the energy spectrum and the wave function of the electron essentially change. A numerical calculation of the thermoelectric power is carried out for the quantum wire $GaAs/Al_xGa_{1-x}As$ with a parabolic well.

## 2. THEORETICAL DETAILS

To obtain an analytical expression for various physical quantities, it is advisable to use a specific model of a potential quantum well. For this purpose, a parabolic potential of the $U(x) = m\omega_0^2 x^2/2$ form that restricts the motion of electrons in the direction of the $x$-axis, is often used, where $m$ is the effective mass of the conduction electrons, and $\omega_0$ is the parabolic potential parameter.

In a present work, the phonon drag thermopower for one-dimensional degenerated electron gas in quantum wire (QW) with a parabolic confinement potential is calculated. Spectrum and wave functions of the system ground state under consideration are given in [5]:

$$\varepsilon_{0,0,k} = \frac{\hbar^2 k^2}{2m} + \hbar\omega, \quad (1)$$

$$\psi_{0,0,k} = \frac{1}{R\sqrt{\pi L}} \exp\left(-\frac{r^2}{2R^2} + ikz\right), \quad (2)$$

where $\omega$ is a parabolic potential parameter, $R = \sqrt{\hbar/(m\omega)}$ is an oscillatory length, $L$ is a QW length. It is supposed that the Fermi level $\zeta$ is localized between zero level and first one of dimensional quantization. Moreover, necessary condition for the existence of a strong degeneration is $k_0 T << \zeta - \hbar\omega < \hbar\omega$, where $T$ is temperature, $k_0$ is the Boltzmann constant. Earlier, the phonon drag thermopower for one-dimensional electron gas was calculated in the framework of the rectangular confinement potential model [6]. There are both theoretical calculations [3, 7] and experimental results [8, 9] confirming the dominating contribution of phonon drag thermopower in the total thermopower for a two-dimensional electron gas.

## 3. RESULTS

Thermopower $\alpha$ associated with a temperature gradient along the QW axis consists of diffusion $\alpha_e$ and phonon $\alpha_{ph}$ parts: $\alpha = \alpha_e + \alpha_{ph} = \beta_e/\sigma + \beta_{ph}/\sigma$ [10]. Here, $\sigma$ is the specific conductivity of the QW along the wire axis:

$$\sigma = \frac{n e^2 \tau(k_F)}{m}. \quad (3)$$

As evaluations show, at low temperatures, the dominating scattering mechanism for strongly degenerated electron gas is scattering on ionized impurities and scattering on a sample boundary for phonons.

The expression for the electron-momentum relaxation time has the form:

$$\tau(k_F) = \frac{1}{N_I}\frac{\hbar^3 k_F}{2m}\left(\varepsilon(k_F)\right)^2\left(\frac{Z\,e^2}{\chi}\exp\left(R^2k_F^2\right)\Gamma\left(0,R^2k_F^2\right)\right)^{-2}; \quad (4)$$

for phonons, $\tau_{ph} = L/s$, where $s$ is the sound velocity in the wire.

The electron concentration $n$ and the Fermi wave number $k_F$ are related by the following expression:

$$n = \frac{2}{\pi}k_F = \frac{2}{\pi\hbar}\sqrt{2\,m(\zeta - \hbar\,\omega)}\,, \quad (5)$$

$$\varepsilon(k_F) = 1 + \frac{2\,m\,e^2}{\pi\hbar^2 k_F\chi}\exp(2R^2k_F^2)\Gamma(0,2R^2k_F^2), \quad (6)$$

where $\varepsilon(k_F)$ is the dielectric function, $\chi$ is the static dielectric constant, $\Gamma(0, x)$ is the incomplete gamma function,

$$\beta_e = -\frac{1}{e\,T}\frac{\pi^2}{3}(k_0T)^2\frac{\partial\sigma}{\partial\zeta}, \quad (7)$$

$$\beta_{ph} = -\frac{k_0}{e}\sigma\,A_{ph}, \quad (8)$$

$$A_{ph} = \frac{4\,m^2e^2\beta^2L\,s\,k_F}{\pi\hbar\rho\left(k_0T\,\varepsilon(k_F)\right)^2}\int_0^\infty(1 + a^2(1 + x^2))\exp(-2\,R^2\,k_F^2\,x^2)\times$$
$$\times(\exp(b\sqrt{1 + x^2}) - \exp(-b\sqrt{1 + x^2}))^{-2}x\,dx, \quad (9)$$

where the following notations are introduced:

$$a = \frac{2\,k_F E_1}{e\beta},\ \ b = \frac{\hbar\,s\,k_F}{k_0T}. \quad (10)$$

Here. $e$ is the elementary charge, $E_1$ is the deformation-potential constant, and $\beta$ is the parameter characterizing the piezo acoustic potential.

The contributions from electron interactions with acoustic phonons in the phonon drag thermopower are taken into account in [9] by means of the deformational potential $E_1$ and the piezo-acoustic one $\beta = \sqrt{0.8\,e_{14}/\chi}$ [11].

## 4. DISCUSSION

Numerical calculations are performed for the GaAs/$Al_xGa_{1-x}$As QW

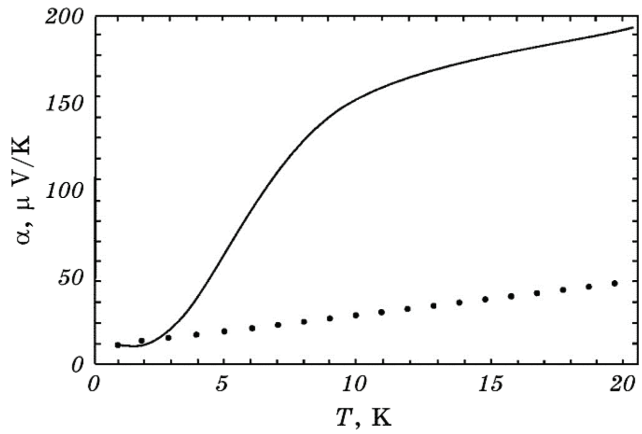


**Fig. 1.** Temperature dependences of the phonon drag thermopower (solid line) and the diffusion thermopower (dotted line).

with the following GaAs parameter values: mass of electrons $m = 0.067\ m_0$, where $m_0$ is the free-electron mass, the crystal mass density $\rho = 3.3 \cdot 10^4$ kg/m$^3$, $s = 5 \cdot 10^5$ m/s, $E_1 = 7.4$ eV, $e_{14} = 0.16$ C/m$^3$, the QW length $L = 3 \cdot 10^{-4}$ m, the linear density of electrons $n = 1.6 \cdot 10^8$ m$^{-1}$, $\omega = 7 \cdot 10^{13}$ s$^{-1}$.

The calculated temperature dependence of the phonon drag thermopower (a solid line) is shown in Fig. 1. For comparison, the temperature-dependent thermopower diffusion component (a dotted line) is also given. The parabolic potential parameter for GaAs/$Al_xGa_{1-x}$ As is inversely proportional to the wire thickness $\hbar\omega = 14.6$ eV$/d(E)$ [12]. Our choice corresponds to thicknesses of about 100 Å.

The diffusion thermopower component value is larger than the phonon one in the temperature interval 1–20 K. The phonon drag strongly

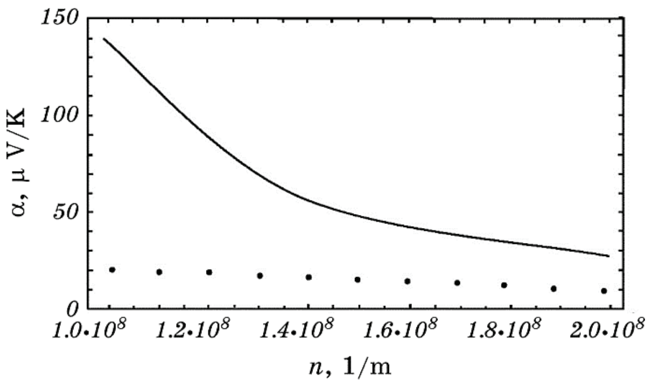


**Fig. 2.** Concentration dependences of the phonon drag thermopower (solid line) and the diffusion thermopower (dotted line).

grows with temperature increasing, exceeding the diffusion thermopower by one order.

The concentration dependences of the phonon drag thermopower (a solid line) and the diffusion thermopower (a dotted line) are shown in Fig. 2. The diffusion component of the thermopower is approximately inversely proportional to the concentration and phonon component is inversely proportional to the concentration squared.

Kubakaddi's expression for the phonon drag thermopower for the QW model with a rectangular potential [6] differs from our expression, but both qualitative results are similar.

## 5. CONCLUSION

The theoretical results obtained are applied to the analysis of a thermopower with phonon drag of a one-dimensional degenerate electron gas in a quantum wire with a parabolic confinement potential. For comparison, the temperature dependence of the diffusion component of the thermoelectric power is also given. Numerical calculations are given for the QW GaAs/$Al_xGa_{1-x}As$. In the temperature range 1–2 K, the diffusion thermoelectric power exceeds the phonon one. With temperature increasing, the phonon thermoelectric power increases sharply, exceeding the diffusion one by an order of magnitude. The diffusion component of the thermoelectric power is approximately inversely proportional to the concentration, and the phonon component is inversely proportional to the concentration squared. In the temperature range 2–20 K, the main contribution to the thermoelectric power is given by the phonon drag.

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