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RELAXATION PROCESSES IN A QUANTUM WIRE WITH PARABOLIC CONFINEMENT

Analytical expressions are found for the mobility of a degenerate electron gas in a quantum wire for three scattering mechanisms: on ionized impurities and on piezoacoustic and deformation acoustic phonons. The expressions allow one to analyze the concentration, temperature, and dimensional dependences of the electron mobility.

Keywords: mobility of a two-dimensional electron gas, quantum wire, elastic scattering by ionized impurities, scattering by acoustic phonons, parabolic confinement potential.

1. Introduction

Currently, the electrotransport phenomena in low-dimensional systems is a subject of intense studies both experimental and theoretical. The practical interest in studying the equilibrium properties and electrotransport phenomena in nanoscale systems is associated with extensive possibilities of their usage for applications. The mobility of current carriers is one of the most discussed characteristics of low-dimensional electron systems.

The carrier mobility in semiconductor nanographenes for the scattering by acoustic phonons, scattering on impurities, and interface roughness scattering was theoretically investigated in Ref. [1]. The impact of thickness fluctuations on the mobility of electrons and the static electrical conductivity of quantum wires was investigated in Ref. [2]. It has been shown that the considered charge carrier relaxation mechanism is essential for the electrical conductivity of a sufficiently thin pure quantum wire (QW) at low temperatures. In Ref. [3], the features, which appear in the mobility in the presence of external electric and magnetic fields, have been revealed.

The mobility of a two-dimensional electron gas at the boundary of $LaAlO_3/SrTiO_3$ at a low temperature was calculated in [4], where it was assumed that the charged impurity scattering dominates. Neglecting the spin-orbital splitting, it was found out that the mobility varies inversely to the cube of the carrier concentration, which agrees well with the experimental results. The transport properties of electron gases located on the boundaries between $SrTiO_3$ and various polar perovskites were discussed, enabling individually to change the epitaxial deformation and charge transfer between these epitaxial interfaces [5]. It was shown that the reduced charge transfer at the boundaries yields a systematic increase in the mobility of electrons, while the reduced epitaxial strain has only a minor impact.

The aim of the paper is to obtain analytical expressions for the mobility of a degenerate quasi-one-dimensional electron gas in a QW for three scattering mechanisms: scattering by ionized impurities, scattering by piezoacoustic and deformation acoustic phonons.

2. Theory

Let us consider a semiconductor QW in the form of a circular cylinder. The radius of the QW base L_x is much smaller than its length L_z , i.e., $L_x \ll L_z$, and the wire is oriented along the z axis. It is known that the Hamiltonian of a quasi-one-dimensional QW for a degenerate electron gas with a parabolic confinement potential has the form

$$\hat{H} = \frac{1}{2m}\mathbf{P}^2 + \frac{1}{2}m\omega^2\left(x^2 + y^2\right). \tag{1}$$

Here, $U(x, y) = \frac{1}{2}m\omega^2(x^2 + y^2)$ is the parabolic potential limiting the electron motion.

The eigenvalues of the energy of Hamiltonian (1) are as follows [6]:

$$\varepsilon_{N,N',k} = \frac{\hbar^2 k^2}{2m} + (N + N' + 1)\hbar\omega. \tag{2}$$

The eigenfunctions corresponding to the energy of electrons (2) have the form

$$\psi_{N,N',k}(x,\, y,\, z) = \frac{1}{\sqrt{L_z}}\varphi_N(x)\,\varphi_{N'}(y)\, e^{ikz}, \tag{3a}$$

where

$$\varphi_N(x) = \frac{1}{\sqrt[4]{\pi}\sqrt{R}\sqrt{2^N N!}}\, e^{-\left(\frac{x}{\sqrt{2}R}\right)^2}\mathrm{H}_N\left(\frac{x}{R}\right). \tag{3b}$$

The function $\phi_{N'}(y)$ has a similar form. Here, $\omega = \sqrt{\frac{k}{m}}$ is the cyclic frequency determined from the parameter of the parabolic potential, $\mathrm{H}_N\left(\frac{x}{R}\right)$ are the Hermite polynomials, $R = \sqrt{\frac{\hbar}{m\omega}}$ is the "length of the oscillator", by analogy with the term "magnetic length".

We have considered the electron scattering mechanisms such as the ionized impurities scattering, acoustic phonons scattering via the deformation and piezoelectric potentials (the case of DA scattering was previously considered in Ref. [7], but without screening).

The analysis of the results for most experiments in quantum systems shows that electrons fill the lowest energy level ($N = 0$) [8]. Therefore, hereinafter, we will consider the situation of the quantum limit, when only one subzone is occupied ($N = N' = 0$).

2.1. Scattering by ionized impurities

The expression for the inverse relaxation time in the approximation for the elastic scattering on ionized impurities has the form [9]:

$$\frac{1}{\tau_I} = 2\sum_{k'} W(0, k', 0, k)\left(1 - \frac{k'}{k}\right), \tag{4a}$$

where

$$W(0,\, k',0,\, k) = \frac{2\pi}{\hbar}N_I\,|\tilde{M}_{0k',0k}|^2\delta(\varepsilon_{0k'} - \varepsilon_{0k}). \tag{4b}$$

Here, W is the electron transition probability from the state k to a state k' as a result of the scattering, and N_I is the impurity concentration. The transition probability amplitudes for a quantum mechanical system from one state to another one are mainly described by the matrix elements

$$\tilde{M}_{0k',0k} = M_{0k',0k}(1 + M^{e-e}_{0k',0k}\Pi(0,0)^{-1}\tilde{M}_{0k',0k} = \\ = M_{0k',0k}(1 + M^{e-e}_{0k',0k}\Pi(0,0)^{-1}, \tag{5a}$$

$$M_{0k',0k} = Z\iiint \psi^*_{0k'}(x,y,z)V(x,y,z)\times \\ \times\psi_{0k}(x,y,z)dxdydz, \tag{5b}$$

$$M^{e-e}_{k_1'k_2',k_1k_2} = \int\int\psi^*_{0k_1'}(\mathbf{r}_1)\int\psi_{0k_1}(\mathbf{r}_1)\times \\ \times V(\mathbf{r}_1 - \mathbf{r}_2)\psi^*_{0k_2'}(\mathbf{r}_2)\psi_{0k_2}(\mathbf{r}_2)d\mathbf{r}_1 d\mathbf{r}_2, \tag{5c}$$

where

$$V(x,y,z) = \frac{e^2}{\chi}(x^2 + y^2 + z^2)^{-1/2}$$

and

$$\Pi(0,0) = \int\limits_{\varepsilon_0}^{\infty}\rho(\varepsilon)\left(-\frac{\partial f_0}{\partial\varepsilon}\right)d\varepsilon.$$

The parameter χ_0 is the static dielectric constant, Z is the impurity charge, $\Pi(0,0)$ is the polarization operator involving the screened Coulomb potential of the impurity [10], $\rho(\varepsilon)$ is the density of states, and $f_0(\varepsilon)$ is the Fermi distribution function.

With regard for Eqs. (1) and (2), Eq. (5) yields

$$M_{0k',0k} = \frac{Ze^2}{\chi L_z} \exp\left(\frac{1}{4} R^2 \left(k' - k\right)^2\right) \times$$
$$\times \Gamma\left(0, \frac{1}{4} R^2 \left(k' - k\right)^2\right), \tag{6a}$$

$$M^{e-e}_{k_1' k_2', k_1 k_2} = \frac{e^2}{\chi L_z} \exp\left(\frac{1}{2} R^2 \left(k_1' - k_1\right)^2\right) \times$$
$$\times \Gamma\left(0, \frac{1}{2} R^2 \left(k_1' - k_1\right)^2\right) \delta_{k_1' - k_1, k_2 - k_2'}, \tag{6b}$$

where $\Gamma(0, x)$ is the incomplete gamma function [11].

It follows from the conservation law that $k' = -k$. Herewith, the inverse relaxation time reads

$$\frac{1}{\tau_I} = L_z \frac{2m}{\hbar^3 k} N_I \times$$
$$\times \frac{\left(\frac{Ze^2}{\chi L_z} \exp\left(R^2 k^2\right) \Gamma\left(0, R^2 k^2\right)\right)^2}{\left(1 + \frac{e^2}{\chi L_z} \exp\left(2R^2 k^2\right) \Gamma\left(0, 2R^2 k^2\right) \Pi\left(0, 0\right)\right)^2}. \tag{7}$$

The mobility of electrons in a degenerate electron gas scattered by ionized impurities in a QW is

$$\mu_I = \frac{e\hbar^3 \pi n}{4m^2 N_I} \times$$
$$\times \frac{\left(1 + \frac{e^2}{\chi} \exp\left(\frac{1}{2} R^2 \pi^2 n^2\right) \Gamma\left(0, \frac{1}{2} R^2 \pi^2 n^2\right) \frac{4m}{\pi^2 \hbar^2 n}\right)^2}{\left(\frac{Ze^2}{\chi} \exp\left(\frac{1}{4} R^2 \pi^2 n^2\right) \Gamma\left(0, \frac{1}{4} R^2 \pi^2 n^2\right)\right)^2}. \tag{8}$$

Here, we set $L_z = 1$ and used the fact that $k_{\rm F} = \frac{\pi n}{2}$ and $\Pi(0,0) = \rho(\varepsilon_{\rm F}) = \frac{4m}{\pi^2 \hbar^2 n}$.

The criterion of strong degeneracy is: $n \gg \gg \frac{2\sqrt{2mk_0 T}}{\pi\hbar}$. On the other hand, since we limited to the ground state, we have a restriction on the concentration $n \ll \frac{2\sqrt{2}}{\pi R}$.

2.2. Scattering by piezoacoustic phonons

Let us now consider the scattering of electrons by piezoacoustic phonons. The piezoacoustic scattering potential has the form [9]:

$$V\left(x, y, z\right) = \frac{eE_{pz}\sqrt{k_0 T}}{\chi\sqrt{\rho\Omega} s} \sum_{\mathbf{q}} \frac{\exp(i\mathbf{qr})}{q}. \tag{9}$$

Taking (3) and (6) into account, the expression for the matrix element of the scattering process under consideration is written as follows:

$$M_{0k',0k} = \frac{L_x L_y}{\pi} \frac{eE_{pz}\sqrt{\pi k_0 T}}{\chi_0 \sqrt{\rho\Omega} sR} \exp\left(\frac{1}{4} R^2 \left(k' - k\right)^2\right) \times$$
$$\times \left(1 - \text{erf}\left(\frac{1}{2} R \left|k' - k\right|\right)\right). \tag{10}$$

Here, $\text{erf}(x)$ is the probability integral [11], E_{pz} is the piezoelectric constant, Ω is the volume, ρ is the density, s is the speed of sound, and k_0 is the Boltzmann constant.

For the relaxation time, we obtain:

$$\frac{1}{\tau_{PA}} = L_z \frac{4m}{\hbar^3 k} \times$$
$$\times \left(\frac{\frac{L_x L_y}{\pi} \frac{eE_{pz}\sqrt{\pi k_0 T}}{\chi\sqrt{\rho\Omega} s} \exp\left(R^2 k^2\right) \left(1 - \text{erf}\left(Rk\right)\right)}{1 + \frac{e^2}{\chi L_z} \exp\left(2R^2 k^2\right) \Gamma\left(0, 2R^2 k^2\right) \Pi\left(0, 0\right)}\right)^2. \tag{11}$$

Respectively, the mobility for a degenerate electron gas scattered by piezoacoustic phonons has the form

$$\mu_{PA} = \frac{e\hbar^3 \pi n}{8m^2} \times$$
$$\times \left(\frac{1 + \frac{e^2}{\chi} \exp\left(\frac{1}{2} R^2 \pi^2 n^2\right) \Gamma\left(0, \frac{1}{2} R^2 \pi^2 n^2\right) \frac{4m}{\pi^2 \hbar^2 n}}{\pi R \frac{eE_{pz}\sqrt{\pi k_0 T}}{\chi\sqrt{\rho\Omega} s} \exp\left(\frac{1}{4} \pi^2 R^2 n^2\right) \left(1 - \text{erf}\left(\frac{1}{2} \pi R n\right)\right)}\right)^2. \tag{12}$$

2.3. Scattering by acoustic phonons

Finally, let us examine the scattering of electrons by acoustic phonons through the deformation potential of an acoustic wave. The interaction potential for this scattering mechanism has the form [9]

$$V(x, y, z) = \frac{E_1 \sqrt{k_0 T}}{\sqrt{2\rho\Omega} s} \sum_{\mathbf{q}} \exp(i\mathbf{qr}). \tag{13}$$

Here, E_1 is the deformation potential. Hence, for the matrix element, we obtain

$$M_{0k',0k} = \frac{L_x L_y}{\pi R^2} \frac{E_1 \sqrt{k_0 T}}{\sqrt{2\rho\Omega} s}. \tag{14}$$

For the inverse relaxation time, we have

$$\frac{1}{\tau_{PA}} = L_z \frac{4m}{\hbar^3 k} \times$$

$$\times \left(\frac{\frac{L_x L_y}{\pi R^2} \frac{E_1 \sqrt{k_0 T}}{\sqrt{2\rho\Omega s}}}{1 + \frac{e^2}{\chi L_z} \exp\left(2R^2k^2\right) \Gamma\left(0, 2R^2k^2\right) \Pi\left(0,0\right)} \right)^2. \quad (15)$$

The mobility for a degenerate electron gas scattered by deformation acoustic phonons takes the following form:

$$\mu_{PA} = \frac{e\hbar^3 \pi n}{8m^2} \times$$
$$\times \left(\frac{1 + \frac{e^2}{\chi} \exp\left(\frac{1}{2}R^2\pi^2n^2\right) \Gamma\left(0, \frac{1}{2}R^2\pi^2n^2\right) \frac{4m}{\pi^2\hbar^2 n}}{\frac{\pi E_1 \sqrt{k_0 T}}{\sqrt{2\rho\Omega s}}} \right)^2. \quad (16)$$

In view of all three scattering mechanisms considered above, the inverse mobility of the electrons is determined, by summing the inverse mobility of the individual scattering mechanisms.

3. Conclusion

Analytical expressions for the mobilities of a degenerate electron gas in a quantum wire for three scattering mechanisms (scattering by ionized impurities, scattering by piezoacoustic and deformation acoustic phonons) have been derived. The obtained expressions allow one to analyze the concentration, temperature, and size dependence of the electron mobility.

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РЕЛАКСАЦІЙНІ ПРОЦЕСИ
В КВАНТОВОМУ ДРОТІ З ПАРАБОЛІЧНИМ
УТРИМАННЯМ

Р е з ю м е

Знайдено аналітичні формули для рухливості виродженого електронного газу в квантовому дроті за трьома механізмами розсіювання: на іонізованих домішках і п'єзоакустичних і деформаційних акустичних фононах. Формули дозволяють аналізувати залежності рухливості електронів від концентрації, температури і розмірності.