Thermoelectric ionization of $D^{(-)}$-centers in a semiconductor quantum wire with a parabolic confinement potential in a strong longitudinal electric field

A B Grunin and I A Kirillov
Penza State University, 40 Krasnaya str., Penza, 440026, Russia
E-mail: kirillov.ia1990@yandex.ru

Abstract. Conductivity of a semiconductor quantum wire with a parabolic confinement potential was studied within the framework of the zero-range potential model, containing donor impurities, in the longitudinal with respect to its axis electric field at low temperatures. A dispersion equation determining the dependence of the binding energy of the impurity on the electric field strength was obtained. It has been shown that the bound state of an electron on an impurity is destroyed by a strong electric field, i.e. the thermoelectric phenomenon of ionization occurs. It was found that under conditions of low temperatures the dependence of the current density in a quantum wire in the longitudinal electric field has a superlinear character.

1. Introduction
At the present time the range of investigated nanostructures is being significantly increased: from quantum wells, quantum dots, quantum cylinders, quantum wires, quantum channels, nanospheres, fullerenes to carbon based nanotubes, graphene, thready nanocrystals [1]. The expansion and complication of subjects of theoretical and experimental works in this area is associated with the desire to understand the depth of quantum processes in nanostructures, as well as with the ability to create new semiconductor optoelectronic and nanoelectronic devices.

The purpose of this work is to theoretically study the phenomenon of the ionization of donor impurity centers ($D^{(-)}$-centers) in a quantum wire (QWire) with a parabolic confinement potential and conductivity of QWire in a strong longitudinal (along its axis) electric field.

There are a lot of studies in which scientists investigate transport and optical properties of semiconductor nanostructures in low electric fields [1,2,3], but the influence of impurities and strong electric fields has been researched to a much lesser extent. There are many simultaneous effects in bulk semiconductors in a strong electric field, such as the Frenkel effect, the Zener effect, impact ionization, etc. [4]. However, these effects have not been sufficiently studied in nanostructures. This fact explains the relevance of the present study.

2. Models
In this paper, we consider cylindrical QWire with a length $L_z$ and a diameter $L$. The electric field strength $\mathbf{F}$ is directed along the axis of QWire. To describe one-electron states in QWire we use the confinement potential in the form of a spherical oscillator well:
For a theoretical description of single-electron states in a quantum wire, various models of the confinement potential are used in the literature: an infinite waveguide with a constant cross section [3, 5, 6], the potential of the saddle point for the restrictions in quantum channels [3, 7, 8], as well as a symmetrical quadratic potential [3, 9, 10]. In a closer approximation of the confining potential shape it is necessary to find self-consistent solutions of the Poisson equation and the Schrödinger equation. The numerical solution of these equations gives results close to the parabolic potential for the channels in a two-dimensional gas but with a flat lower boundary (with the lower part cut off [10]). Since this form of the potential is very close to parabolic, the harmonic potential corresponds to the experimental results [9].

Practical implementation of the transversal parabolic potential can be performed by introducing impurities into QWire and barrier layers, similar to the case of multiwell quantum structures. Also, the restriction can be implemented by the influence of an external magnetic field [11].

As is well known [4], the contact potential difference occurs upon the metal-semiconductor contact and is proportional to the square of the width of the barrier layer. Therefore, the confining potential along the axis of QWire is also similar to a parabolic one, but with the lower part cut off.

Wave functions and energy spectrum of an electron in QWire with an external longitudinal electric field, respectively, have the form:

\[
\psi_{n_1,n_2,n_3}(x,y,z) = \frac{1}{\sqrt{\pi a^3}} H_n\left(\frac{x}{a}\right) H_n\left(\frac{y}{a}\right) H_n\left(\frac{z-z_0}{a_z}\right) \exp\left(-\frac{x^2 + y^2}{2a^2} - \frac{(z-z_0)^2}{2a_z^2}\right),
\]

\[
E_{n_1,n_2,n_3} = \hbar \omega_n\left(n_1 + 1\right) + \hbar \omega_n\left(n_2 + 1\right) + \hbar \omega_n\left(n_3 + 1\right) - \frac{e^2 F^2}{2m^* \omega_n^2},
\]

where \( n_1,n_2,n_3 = 0,1,2,... \) are oscillator quantum numbers; \( a = \sqrt{\hbar / (m^* \omega)} \) is the characteristic length of the oscillator along the axis \( OX \) (or \( OY) \); \( a_z = \sqrt{\hbar / (m^* \omega_z)} \) is the characteristic length of the oscillator along the axis \( OZ \); \( H_n(x) \) are Hermite polynomials [12]; \( z_0 = |e|F / (m^* \omega_z^2) \); \( e \) is the electron charge; \( F \) is the electric field strength.

The confining potential of QWire must have a finite depth. Thus, the amplitude of the confining potential \( V \) (1) is an empirical parameter. The value of the confining potential amplitude along the axis \( OX \) (or \( OY) \) is equal to \( V_{OY} = m^* \omega_x^2 L_x^2 / 8 \); along the axis \( OZ \) - \( V_{OZ} = m^* \omega_z^2 L_z^2 / 8 \). Therefore, expressions (2) and (3) are valid when \( V_{OY} / (\hbar \omega) >> 1 \) and \( V_{OZ} / (\hbar \omega) >> 1 \).

Let us consider \( D(i)- \) center localized at the point \( \vec{R}_a = (x_a, y_a, z_a) \). The impurity potential is modeled by the zero-range potential [13] with the intensity \( \gamma = 2\pi \hbar^2 / (\alpha m^*) \). In the Cartesian system of reference, this potential can be written as:

\[
V_i(\vec{r}, \vec{R}_a) = \gamma \delta(x-x_a) \delta(y-y_a) \delta(z-z_a) \left[ 1 + (x-x_a) \frac{\partial}{\partial x} + (y-y_a) \frac{\partial}{\partial y} + (z-z_a) \frac{\partial}{\partial z} \right],
\]
where $\alpha$ is determined by the binding energy $E_i = -\hbar^2 \alpha^2 / (2m^*)$ for the same $D^+\beta$-center in a massive semiconductor; $\delta(x)$ is the Dirac delta-function.

3. Calculations

The wave function $\Psi_{QWire}^{QWire}(\vec{r}, \vec{R})$ for the electron which is localized at the $D^+\beta$-center, in the effective mass approximation, satisfies the Schrödinger equation:

$$\left(E_\lambda - \hat{H}\right) \Psi_{QWire}^{QWire}(\vec{r}, \vec{R}) = \left(\nabla^2 + V_\delta(\vec{r}, \vec{R})\right) \Psi_{QWire}^{QWire}(\vec{r}, \vec{R}),$$

(5)

where $\hat{H}$ is the Hamiltonian operator; $E_\lambda = \hbar^2 \lambda^2 / 2m^*$ are eigenvalues of the Hamiltonian $\hat{H}_\delta = \hat{H} + V_\delta(\vec{r}, \vec{R})$.

Equation (5) is solved by the method of Green-functions. The one-electron Green-function $G(r, \vec{r}_i, E_\lambda)$ associated to the Schrödinger equation (5) corresponding to the energy $E_\lambda$ and to the source at the point $\vec{r}_i = (x_i, y_i, z_i)$, can be written as:

$$G(r, \vec{r}_i, E_\lambda) = \sum_{n_1, n_2, n_3} \frac{\Psi^*_{n_1, n_2, n_3}(\vec{r}_i) \Psi_{n_1, n_2, n_3}(\vec{r}_i)}{E_\lambda - E_{n_1, n_2, n_3}}.$$

(6)

The Lippman-Schwinger equation for $D^+\beta$-state in QWire in an external electric field is:

$$\Psi_{QWire}^{QWire}(\vec{r}, \vec{R}) = \int d\vec{x}_1 d\vec{y}_1 d\vec{z}_1 G(r, \vec{r}_i, E_\lambda) \nabla^2 \Psi_{QWire}^{QWire}(\vec{r}_i, \vec{R}_i) \Psi_{QWire}^{QWire}(\vec{r}, \vec{R}).$$

(7)

By substituting the expression for zero-range potential (4) into equation (7) we obtain:

$$\Psi_{QWire}^{QWire}(\vec{r}, \vec{R}) = \gamma G(r, \vec{r}_i, E_\lambda) \left(\hat{T} \Psi_{QWire}^{QWire}(\vec{r}, \vec{R})\right)\left(\vec{R}_i, \vec{R}_o\right),$$

(8)

where:

$$\left(\hat{T} \Psi_{QWire}^{QWire}(\vec{r}, \vec{R})\right)\left(\vec{R}_i, \vec{R}_o\right) = \lim_{\vec{R}_d \to \vec{R}_o} \left(1 + (x - x_o) \frac{\partial}{\partial x} + (y - y_o) \frac{\partial}{\partial y} + (z - z_o) \frac{\partial}{\partial z}\right) \Psi_{QWire}^{QWire}(\vec{r}, \vec{R}).$$

(9)

The equation which determines the dependence of the binding energy of $D^+\beta$-center on the parameters of QWire, the position $\vec{R}_o = (x_o, y_o, z_o)$ of the impurity, and the electric field strength $\vec{F}$ can be obtained by applying the operator $\hat{T}$ to the left and right hand sides of equation (8). This gives us:

$$\alpha = \frac{2\pi \hbar^2}{m^*} \left(\hat{T} G\right)(x_o, y_o, z_o, x_o, y_o, z_o, E_\lambda).$$

(10)

By summing the terms of the right side of equation (6) over the quantum numbers $n_1, n_2, n_3$, we obtain the one-electron Green-function with a distinguished divergent part [12]:

$$G(r, \vec{R}_o, \beta, \beta, \eta) = C(\vec{R}_o) \int_0^\infty \frac{1}{1 - \exp(-2\beta t)} \left(1 - \frac{1}{1 - \exp(-2\beta t)}\right) \times
\exp\left(\frac{2\exp(-\beta t)(x^2 + y^2 + z^2) - \exp(-2\beta t)(x_o^2 + y_o^2 + z_o^2)}{a^2(1 - \exp(-2\beta t))}\right) \times$$

$$\times \hat{T} G(x_o, y_o, z_o, x_o, y_o, z_o, E_\lambda).$$
\[
\begin{align*}
\times & \exp \left\{ \frac{2\exp(-\beta t)(z_a - z_0)(z - z_0) - \exp(-2\beta t)\left((z_a - z_0)^2 + (z - z_0)^2\right)}{a_z^2\left(1 - \exp(-2\beta t)\right)} \right\} dt - \\
& - \frac{1}{2\beta \sqrt{2\beta} a_z^2} \int_0^\infty \exp(-bt) \exp \left\{ -\frac{1}{t} \left( \frac{(x - x_a)^2 + (y - y_a)^2 + (z - z_0)^2}{2a^2} \right) \right\} t^{-3/2} dt + \\
& + \sqrt{\frac{\pi}{2\beta^3 a_z^2}} \sqrt{\frac{a^2}{a_z^2}} \exp \left\{ \frac{-\sqrt{2b}}{a_z^2} \left( \frac{1}{a^2} \left( (x - x_a)^2 + (y - y_a)^2 + (z - z_0)^2 \right) \right) \right\}.
\end{align*}
\]

where
\[
C(\vec{r}, \vec{R}_0) = -\frac{\beta \beta_i z}{\pi^{3/2} E_d a_z^2} \exp \left\{ -\frac{x^2 + x_a^2 + y_a^2 + y^2}{2a^2} - \frac{(z_a - z_0)^2 + (z - z_0)^2}{2a_z^2} \right\}; \quad \beta = \hbar \omega / E_d;
\]

\[\beta_i = h\omega / E_d; \quad E_d \quad \text{the effective Bohr energy}; \quad b = (E_D / E_d) \beta \beta_i = \eta^2 \beta z + \beta z + \beta / 2 \; ; \quad E_D = E_{0,0,0} - E_i \quad \text{the binding energy of the D}^i\text{-state}; \quad \eta^2 = |E_i| / E_d.\]

By substituting (11) from (10) we obtain the dispersion equation for the D\(^{-}\)-state of the electron in QWire with the influence of a strong longitudinal electric field:
\[
\sqrt{|E_i|} = \frac{\sqrt{2}\pi a_z}{m} \frac{\sqrt{\pi b}}{\beta \sqrt{2\beta} a_z^2} + C(\vec{r}_z, \vec{R}_0) \int_0^\infty \exp(-bt) \left\{ \frac{1}{(1 - \exp(-2\beta t))(1 - \exp(-2\beta t))} \right\} \times \\
\times \exp \left\{ \frac{2(x^2 + y^2)}{a^2(1 + \exp(-\beta t))} \frac{2(z_a - z_0)^2 \exp(-\beta t)}{a_z^2(1 + \exp(-\beta t))} \right\} \frac{1}{2\beta_i \sqrt{2\beta}} dt.
\]

4. Results

Figures 1 and 2 show the results of numerical analysis of the dispersion equation (12) which determines the dependence of the binding energy \(E_D\) of D\(^{-}\)-state on the value of the strong longitudinal electric field strength \(\vec{F}\), the parameters of confining potential of QWire, the characteristics of impurity (the power of zero-radius potential \(\gamma\), coordinates \(\vec{R}_u = (x_a, y_a, z_0)\) of the impurity center) in GaAs.

Figure 1 shows that the increase of the electric field strength \(\vec{F}\) leads to a strong decrease of the binding energy \(E_D\) of the impurity state (see curves 1 and 2, figure 1) due to the quantum-confined Stark effect for one-electron states in QWire [14]. Since the wave function of the electron on an impurity is formed from electron states of the conduction band, the displacement of impurity levels in the electric field is similar to the displacement of the energy levels of the electron in the conduction band. However, displacement of the impurity level is much lower in the same electric field than that for the Stark effect for the conductivity band. Therefore, the dynamics of size-quantization levels and impurity level leads to the destruction of the bound state of the electron on an impurity in the electric field, i.e. its ionization at a certain value of the electric field strength \(\vec{F}\) (see curve 1, figure 1). The impurity level is deeper at a higher power of the zero-potential radius \(\gamma\), and, therefore, thermo-electric ionization occurs at higher field strength \(\vec{F}\) (see curve 2, figure 1).

Figure 2 shows the dependence of the binding energy \(E_D\) of D\(^{-}\)-state on the coordinates \(x_a\) (or \(y_a\)) of an impurity in QWire of GaAs. The decrease of the binding energy \(E_D\) when approaching the boundary of QWire is due to the influence of the confinement potential. This effect is known as a
"position disorder effect" [15]. A comparison of curves 1 and 3 in figure 2 shows that the region of existence of impurity states decreases with increase of the electric field strength $\vec{F}$ "pulling" to the axis of the QWire, and at a certain value of the electric field strength the bound states do not occur.

Thus, the thermoelectric ionization effect, which occurs in QWire with impurities in the strong longitudinal electric field at low temperatures, results in increase of the concentration of free electrons in the conduction band. This effect is called the Frenkel effect in bulk semiconductors [4].

The range of values of the electric field strength $\vec{F}$, which was considered by the thermoelectric ionization effect, is from $2\cdot10^6$ V/m to $2,3\cdot10^6$ V/m. In general, the considered range of values of the electric field strength $\vec{F}$ is determined by the characteristics of impurity centers ($\gamma, R_x$) and the parameters of QWire ($L, L_x, V_0$).

The numerical solution of the equation of electrical neutrality for the impurity conductivity at low temperatures makes it possible to estimate the dependence of the current density $\bar{j}$ on the electric field strength $\bar{F}$ in QWire, provided that the dependence of the electron mobility $\mu$ on the electric field strength $\bar{F}$ is not too strong [16].

Figure 3 shows the dependence of the current density $\bar{j}$ on the electric field strength $\bar{F}$, which has a superlinear character. The sharp increase of current density occurs at a certain value of the electric field strength, which is the closest to the value of the ionization electric field strength, when practically all impurities are ionized. The increase of temperature accelerates the process of ionization (see curves 1 and 3, figure 3). Therefore, the current density increases due to the corresponding dynamics of the Fermi level. Increasing the concentration of impurity centers $N_D$ also leads to an increasing current density (see the curves 2 and 3, figure 3).

**Figure 1.** The binding energy $E_D$ dependence (for $D^{(-)}$-center in QWire, based on GaAs) on the value of the longitudinal electric field strength $F_x$ (curve 3 shows the dependence of ground state energy $E_{0,0,0}$ on $F_x$); $L = 9,1$ nm; $L_x = 91$ nm; $V_{0x} = V_{0y} = 0,2$ eV; $V_{0z} = 0,02$ eV; $x_a = 0$; $y_a = 0$; $z_a = 0$. Curve 1 – $E_i = 2\times10^{-3}$ eV; 2 – $E_i = 9\times10^{-3}$ eV.

**Figure 2.** The binding energy $E_D$ dependence (for $D^{(-)}$-center in QWire, based on GaAs), on the coordinate $x_a$ (or $y_a$); $L = 9,1$ nm; $L_x = 91$ nm; $V_{0x} = V_{0y} = 0,2$ eV; $V_{0z} = 0,02$ eV; $z_a = 0$; $E_i = 9\times10^{-3}$ eV. Curve 1 – $F = 2,1\times10^6$ V/m; $2 – F = 1,6\times10^6$ V/m; $3 – F = 10^7$ V/m.
5. Conclusion

From a fundamental point of view, the considered effect of the thermoelectric ionization in QWire allows us to estimate the binding energy and the concentration of impurities. From a practical point of view, this effect makes it possible to control the concentration of free charge carriers and, hence, electrical conductivity of QWire, that is important to develop new semiconductor nanoelectronic devices [17, 18].

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