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Nonlinear resonant tunneling as mechanism of cool electrons filtration

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The paper is devoted to the explanation of the effect of suppressing the temperature distribution of the current carriers in the tunneling device where a nanoparticle embedded in a dielectric matrix served as a quantum dot (QD). Due to a spatial confinement the quantization of energy takes place in the QD. Each level assumed to be four-fold degenerated. We suppose the existence of the strong electron–phonon interaction in the QD leading to the attraction of electrons that exceeds the Coulomb repulsion. This interaction results in breaking the degeneracy. The discrete levels can have lower energies than the Fermi energy of the electrode. The tunneling current through these levels will not be affected by the temperature. In the proposed mechanism of the cool electrons filtration, fitting parameters are absent and nevertheless a good agreement between the theory and experiment has been achieved.

Keywords: resonant tunneling, quantum dot, electron–phonon interaction, electron energy filtering.

1. Introduction

The thermal distribution of charge carries is the essential limitation for the use of nanoelectronic devices. In such systems with a small number of charge carries (low current) subjected to scattering, the information component may be lost. The solution to this problem was proposed in some papers [1–3] with the help of devices consisting of consecutively connected quantum dots (QD). These two dots act as filters allowing only electrons of certain energy to tunnel through. These devices are called “QD coolers” (or “QD refrigerators”).

In Ref. 4 it was reported about the energy-filtered cold electron transport at room temperature. Cold electron transport was detected from extremely narrow differential conductance peaks with the width at half maximum of 15 mV at room temperature. The device consisted of two electrodes (Cr) that were separated by an insulating layer. A nanoparticle of CdSe (served as QD) embedded in a matrix of SiO_2 was positioned on the insulating layer. At applying an external voltage, a current from a source electrode flows to a drain one through the QD. A thin layer of Cr_2O_3, that was naturally formed on the Cr surface, served as a tunneling barrier.

The authors assumed that an additional quantum well (QW) was formed between Cr_2O_3 and SiO_2 at applying the bias voltage. This configuration forms a three-barrier tunneling system consisting of a successive QW and a QD. In such a system, the peak-wise character of the current dependence on the separation of energy levels in QW and QD is supposed [5].

In our opinion, the authors did not take into consideration some important moments. One of them is the strong local heating of the central barrier that was not taken into account in the analysis. The other is the transformation of the energy spectrum in the QD that can drastically change the passage of charge carriers through the dot [6,7]. When this effect takes place, the process of resonant tunneling can become a nonlinear one. The mechanism of nonlinearity with the strong electron–phonon interaction has been proposed in Refs. 8, 9 and was developed in Ref. 10. It was successfully applied in Ref. 11 for the explanation of the occurrence of the bistability of tunneling when molecules of rhodopsin were used as quantum dots.

In contrast to Ref. 4, we suggest that a nanoparticle sits deeper in the layer Cr_2O_3 so that there is no SiO_2 layer between QD and Cr_2O_3. In this configuration, layers of Cr_2O_3 but not of SiO_2 serve as tunneling barriers. Such a configuration is a more realistic one from the technological point of view because otherwise at the process of conservation the system with SiO_2, the QD cannot be fixed properly. Thus, our system is a conventional double-barrier-tunneling structure having a QD as a central island.

The occurrence of the current steps is the result of resonant tunneling through levels that are formed due to a spatial quantization. We assume that these levels are four-fold degenerated. The important feature of this approach is the breaking of degeneracy of states as a result of the strong electron–phonon interaction in the QD. The split levels can have lower energies than the Fermi energy of the source electrode. Such an approach permits to describe experimentally observed suppressing of temperature smearing in the tunneling structure.

The paper is organized as follows. In Sec. 2 we discuss the energy spectrum of the proposed device. The theoretical background of energy level splitting is presented in Sec. 3. We have shown how the occupancy of the dot differs as a function of a gate voltage in Sec. 4 and a bias voltage in Sec. 5. The comparison of the results of numerical calculations with experimental results of Ref. 4 is given in Sec. 6. The discussion and concluding remarks are presented in Sec. 7.

2. Energy spectrum of a semiconductor QD embedded in a dielectric matrix

Unique properties of nanoparticles embedded in a matrix are due to the confinement of the electron motion to a region comparable to the de Broglie wavelength of the particle. The result is the quantization of energy. The spectrum of a nanoparticle resembles that of the "atom" with *s*-, *p*-, *d*-… levels, and the gap between levels depends on the particle size. Such a particle is called a quantum dot.

As is known from literature [12], discrete energy levels in the volume of size L due to spatial quantization are defined by the relation

$$E(n) = \frac{\pi^2 \hbar^2 n_L^2}{2m_e L^2} + E_{\min}, \tag{1}$$

where $n_L = 0, \pm 1, \pm 2, \ldots$ and m_e is an electron mass. The whole spectrum of a semiconductor particle embedded in a dielectric matrix is shown in Fig. 1. Since the valence band is completely occupied by electrons, then $E_{\min} = \max E_v$, where E_v is the electron energy in the valence band.

As can be seen in Fig. 1, the spectrum of a semiconductor acquires a discrete character. For the lowest allowed state, the quantum number n_g referred as the *s*-state in the experimental work [4] is defined from the condition $E(n_g) = E_g$. Using Eq. (1) we get $n_g = \sqrt{2mE_g}/\pi\hbar$. In a bulk semiconductor CdSe, the width of the forbidden band is $E_g = 1.7$ eV, and according to Ref. 13 for a nanoparticle of the size 5–7 nm its value is approximately of 2 eV. Therefore, we obtain for the *s*-state that $n_g \approx 16$. In the states with $|n_L| > n_g$, when electrons enter the conduction band, the electron mass can take the effective value of $m_e = m_{\text{eff}}$, so the distance between their levels may differ

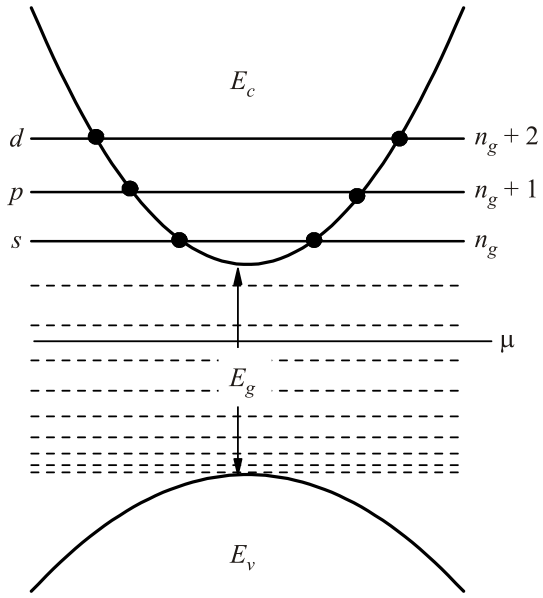

Fig. 1. Energy spectrum of a semiconductor particle embedded in a dielectric matrix. μ is a chemical potential of a semiconductor. E_g, E_v, and E_c are the forbidden, valence, and conduction bands, respectively. The dashed lines correspond to energy states forbidden for electrons.

from energy intervals for the states having numbers within the range of $|n_L| < n_g$.

In the case of the spatial quantization, the distance between energy levels is not a constant value. It depends on the quantum number n_g as follows from Eq. (1):

$$\begin{aligned} \Delta E_1 &= E(n_g + 1) - E(n_g) = \varepsilon_0 (2n_g + 1), \\ \Delta E_2 &= E(n_g + 2) - E(n_g + 1) = \varepsilon_0 (2n_g + 3), \end{aligned} \tag{2}$$

where $\varepsilon_0 = \pi^2 \hbar^2 / 2m_{\text{eff}} L^2$. To define n_g from the experimental data the next relation is useful $\delta = \Delta E_1 / (\Delta E_2 - \Delta E_1) = n_g + 1/2$. According to Ref. 14, in the dependence of the differential current conductivity on the applied bias voltage, the sharp peaks are observed that separated by intervals proportional to the distances between the levels.

In Fig. 2(a) the fragment of such a dependence is demonstrated at temperature $T = 77$ K. As can be seen in Fig. 2(a), the energy distances between *s*–*p* and *p*–*d* levels are different. The estimation of this difference leads to a value $\delta = 18 \pm 2$ being in the interval $15 \le \delta \le 20$ close to the one calculated by the formula (2). From Eqs. (2), the simple formula for the energy distance between the *s*- and *v*-levels is followed:

$$\Delta E_{s-\nu} = 2\nu \sqrt{\varepsilon_0 E_g} + \varepsilon_0 \nu. \tag{3}$$

For $n_g = 18$ and $E_g = 2$ eV we get the value $\varepsilon_0 = 6.2$ meV.

In Fig. 2(b) the calculated dependences (solid lines) of the energy spacings between the levels *s* and *p, d, f* ($\nu = 1, 2, 3$, respectively) on the energy of the forbidden band in the

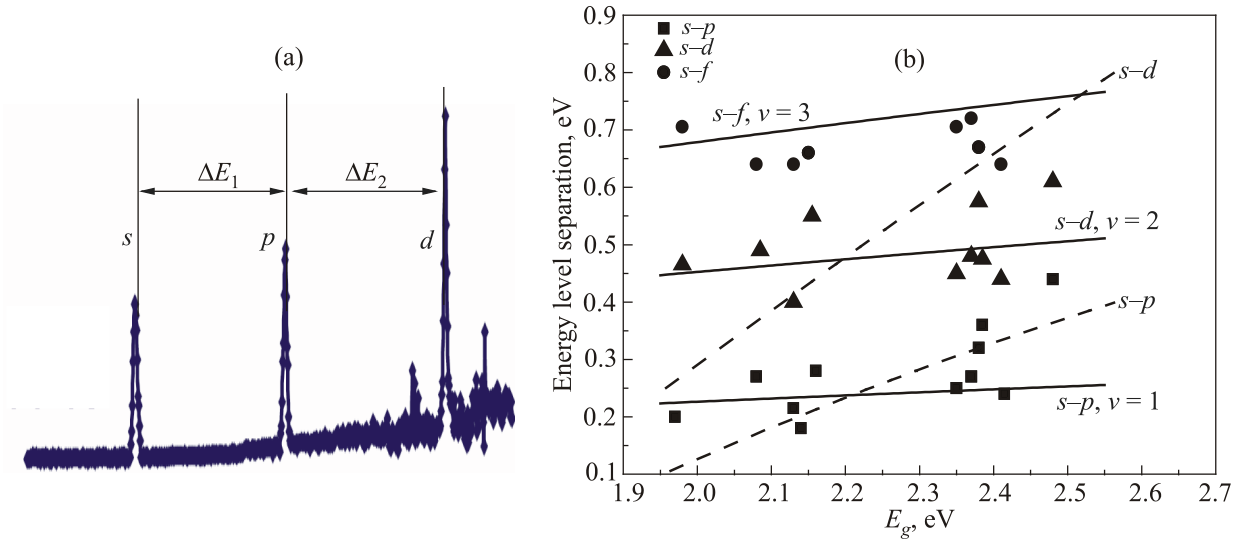

Fig. 2. (*a*) Demonstration of the experimentally observed [4] difference of energy intervals between *s–p* and *p–d* levels ($\Delta E_2 > \Delta E_1$). (b) Energy level separation as a function of the forbidden band energy in QD. Solid lines are calculated using Eq. (3) with $\varepsilon_0 = 6.2$ meV, dashed lines correspond to the model of Coulomb blockade [14], ■, ▲, ● are the experimental data [14].

QD is shown. These dependences are compared with the experimental values given in Ref. 14 and with similar dependences obtained in the model of the Coulomb blockade [14] (dashed lines).

The obtained theoretical relations can be refined with the account of the dependences of ε_0 and E_g on the QD size. As can be seen in the figure, the agreement of the theory with experimental values for the model of the spatial quantization is better than for the model of the Coulomb blockade.

3. Theoretical background

As follows from Fig. 1, the allowed states in the QD are degenerated by a quantum number n_L and spin. So in this case, at least a four-fold degeneracy is possible. When electron–electron interaction or electron–phonon interaction is taking into account, this degeneracy may be removed. To describe this phenomenon we use the approach of Refs. 8, 9 were a four-fold degeneracy of the QD is considered.

According to the method of Ref. 9, to simplify the description we restrict ourselves by the consideration of the current transport through the allowed four-fold degenerate state with the lowest energy level $E(n_g) \equiv E_m$ $(m = 0, 1, 2, 3)$. The electron–phonon interaction removes the degeneracy and the energy E_m will depend on a number m. In this case, the current can be defined by the expression [9]

$$J_{cd} = \frac{e}{\hbar}\sum_{m=0}^{3}\frac{\Gamma_R(E_m)\Gamma_L(E_m)}{\Gamma_R(E_m)+\Gamma_L(E_m)}\times$$

$$\times\{f_L(E_m)-f_R(E_m)\}(1-n)^{3-m}n^m C_3^m + J_s \qquad (4)$$

in which $\Gamma_L(E_m)/\hbar$ and $\Gamma_R(E_m)/\hbar$ are the transfer rates of electron passing through the left and the right barrier, respectively. $f_L(E_m)$, $f_R(E_m)$ are the distribution functions in the left and right electrodes, correspondingly, for electrons they usually have the form of the Dirac function

$$f_{L,R}(E_m) = [\exp((E_m - \mu_{L,R})/kT)+1]^{-1}. \qquad (5)$$

Here $E_m = E_g + mU - \gamma V$ is the energy value of the allowed states in the QD at the applied bias V. In the case of an intrinsic semiconductor $E_g - \mu = E_g/2 = \Delta E$ and $\gamma = a_L/(a_L + a_R)$, where a_L and a_R are the widths of left and right potential barriers, respectively. Under the conditions of the experiment, $a_R \approx a_L$, thus $\gamma = 0.5$. Chemical potentials of the left and right electrodes are connected by the condition $\mu_L = \mu_R + V$. From now on we assume $\mu = \mu_L$. The parameter $U = U_C - U_{\text{ph}}$ defines the amount of splitting of energy levels. It consists of two parts, one is the Coulomb repulsion U_C and the other U_{ph} is due to the interaction of electrons through phonons. The latter interaction results in the attraction of electrons. Current J_s is caused by the passage through other channels, and further will be assumed small enough to be neglected.

In the expression for the tunneling current (4), the main factor that determines the influence of the degeneracy is the electron occupation number n of the energy state after the degeneracy has been removed. This number, according to [9], can be found from the equation

$$n = F(n), \qquad (6)$$

where

$$F(n) = \sum_{m=0}^{3} C_3^m g_m (1-n)^{3-m} n^m, \quad C_m^3 = \frac{3!}{m!(3-m)!},$$

$$g_m = g(E_m), \quad g(E) = \frac{\Gamma_L(E)f_L(E) + \Gamma_R(E)f_R(E)}{\Gamma_L(E)+\Gamma_R(E)}.$$

In the following, we will use the approach in which $\Gamma_L(E_m) = \Gamma_R(E_m) = \Gamma$ are constant values. This approximation is not a critical one but greatly simplifies the analysis and allows to get the correct enough estimations. Also we will neglect the dependence of Γ on the applied bias.

4. Occupancy of the QD as a function of the gate voltage

Let's consider how the occupancy of the split levels of the four-fold degenerate state is changed when its position with respect to the chemical potential of electrodes shifts. For the factor that shifts energy levels in the QD we choose the gate voltage V_g. When the value of V_g is such that $E_m > \mu$ for all m numbers (m = 0, 1, 2, 3), then QD is not filled with electrons and the degeneracy is not removed, as demonstrated in Fig. 3(a). With increasing of the gate voltage, the value of E_1 reaches the value of the chemical potential ($E_1 = \mu$ but $E_0 > \mu$). At that moment the energy level splits abruptly (see Fig. 3(b)).

Every split level will be occupied by electrons, and electron at the level E_0 will have the energy which exceeds the Fermi energy at the value of U. This is reasonable because the whole energy of the system W in this case,

$$W = \sum_{m=0}^{3} (E_m - \mu), \tag{7}$$

is negative.

In the range of the voltage values, $E_1 < \mu < E_2$, according to Eq. (5), the system becomes bistable and may be in three states. The states with occupation numbers of $n_1 = 0$ and $n_2 = 1$ are stable while the state with $n_2 = 0.5$ is unstable. Appearance of bistability is due to the requirement of changing the energy of the QD with the value of U. Therefore, the QD with the negative splitting energy of degenerate states in the case of the four-fold degeneracy can remember the previous value of the gate voltage.

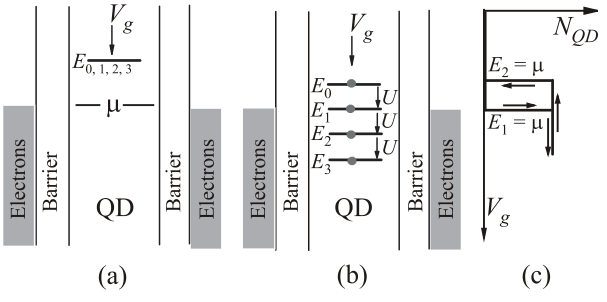

Fig. 3. Dependence of the QD occupation on the mutual position of energy levels with respect to the chemical potential of electrodes. Bias voltage at the gate shifts energy levels of QD by the value of V_g relative to the chemical potential μ: (a) The case when $E_1 > \mu$; (b) Breaking of degeneracy at $E_1 > \mu$; (c) Hysteresis in the dependence of the QD occupation on the bias at the gate.

5. Occupancy of the QD as a function of the bias voltage

When a bias voltage is applied to the QD having a degenerate state and the negative splitting energy, three situations leading to different experimental results are possible. They differ with respect to the original location of the degenerate level relative to the chemical potential. Let's consider four possible cases.

1. $E_m > \mu$ for all m numbers. In this case, we have $f_R(E_m) = 0$ at low temperatures. As follows from Eq. (7) with account of Eq. (6), the simple expression for the tunneling current can be derived

$$J_{cd} = J_0 n, \tag{8}$$

where $J_0 = e\Gamma/\hbar$. Increasing the bias until the condition $E_1 > \mu$ is valid does not lead to the current through the tunnel system and the degeneracy is not removed, as is shown in Fig. 4(a).

2. When the value of the bias reaches the value at which $E_1 \le \mu$, but $E_0 > \mu$, the abrupt splitting of the degenerate level takes place (see Fig. 4(b)) and the current abruptly begins to flow. In this case tunneling occurs through the levels E_1, E_2, and E_3 which are partly filled with electrons. The level with the energy E_0 is not occupied by electrons and does not participate in the electron transport. Those electrons that are transported through the levels E_2, E_3 have the energy significantly low than the Fermi energy and therefore they are cold and are not affected by thermal scattering. That's why we will observe a very abrupt current step with a very small thermal distribution. The contribution to the current due to tunneling through the E_1 level is influenced by temperature. With a further increase in the bias when $E_0 \le \mu$, there will be an additional broad peak and all energy levels will become half filled with electrons.

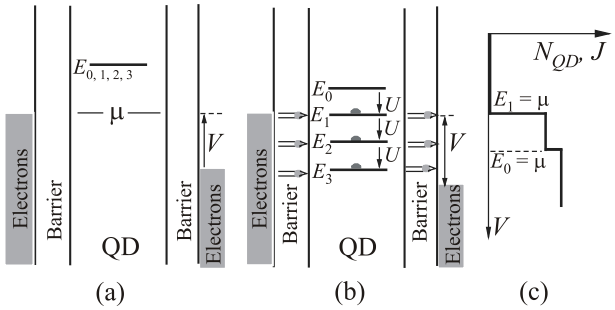

Fig. 4. Dependence of current and QD occupation on the external bias at $E_0 > \mu$. (a) The bias voltage is such that $E_1 > \mu$, there are no splitting and current. (b) When the condition $E_1 < \mu$ is obtained, the abrupt splitting of the degenerate state occurs. Levels in QD are partially occupied by electrons. Current flows through the system. With increasing voltage, the tunneling current grows. (c) Schematic dependence of the current J and the QD occupation N_{QD} on applied bias V.

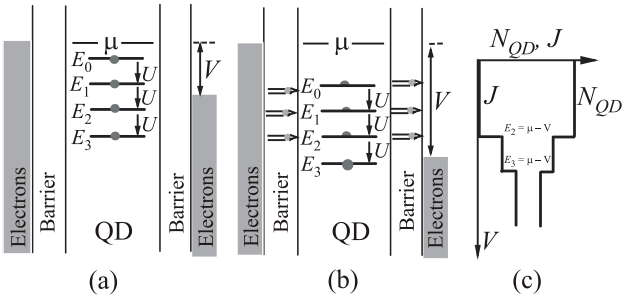

Fig. 5. Current and QD occupation dependence on the bias provided that $E_0 < \mu_L$. (a) If the bias value is such that the condition $E_2 < \mu - V$ is valid, then degenerate states are split and completely filled with electrons. The current does not flow through the system. (b) With increasing the bias provided that $E_2 > \mu - V$, the current will pass through the system. The states with the energies E_0, E_1, E_2 are partially filled. With a further increase in the bias under the condition $E_3 > \mu - V$, the current is increased and all states become partially occupied. (c) Schematic dependence of the current J and the QD occupation N_{QD} on applied bias V.

3. In the case when $E_0 < \mu$ at low temperatures and low bias, we get $f_L(E_m) = f_R(E_m) = 1$ according to Eq. (5), the degeneracy will be removed and all levels in the QD will be occupied by electrons. As the bias grows, the distribution functions $f_R(E_{0,1})$ take the value close to zero. However, electrons are confined to levels E_0, E_1 and block the transport through them as shown in Fig. 5(a). This situation persists until the bias reaches the value that satisfies the condition $E_2 > \mu - V$. Then the occupation of states with $m = 0, 1, 2$ sharply changes, it becomes partial, and resonant tunneling takes place through them as illustrated in Fig. 5(c). The transport begins abruptly because electrons that take part in the process are injected with the energy significantly lower than Fermi energy. The level E_3 is completely filled. With a further growth of the bias when the value $E_3 \geq \mu - V$ is reached, this level also becomes partially occupied and through it the electron transport also begins leading to an additional increase in current as shown in Fig. 5(c).

4. $E_2 < \mu < E_1$. This case is the intermediate one between the two others discussed above. It also can be described on the basis of Eqs. (3) and (5).

6. Broadening of differential conductivity peaks

It is evident that in the experiments with CdSe nanoparticles described in Ref. 4 we deal with the first case considered in the previous section, when we can expect that $E_3 > \mu_L$. At finite temperatures, Eq. (6) can be calculated numerically and with the use of Eq. (7) one can calculate the current and its derivative with respect to the bias in the region of a step in the differential conductivity. In Fig. 6 the results of such a calculation are represented. As can be seen in Fig. 6(a) with the increase of the absolute value of the splitting energy U, the profile of the differential conductivity peak narrows and becomes asymmetric. Temperature dependence of the full width at the half maximum (FWHM) of this peak shown in Fig. 6(b) also varies with increasing of the splitting energy. The width is significantly reduced at the value $U = -0.05$ eV. FWHM values become close to the observed ones [4] when $|U| > 0.2$ eV.

Numerical calculations show that the dependence of the width of the differential conductivity peak on the value of the splitting energy U has an exponential character and can be well described by the relation

$$W = W_0 \exp\left(\frac{U}{b\,kT}\right) + W_{\min}, \qquad (9)$$

where $W_0 + W_{\min}$ is the width of the peak at $U = 0$, i.e., when the degeneracy is not removed, with $b = 4 \pm 0{,}11$ being a dimensionless parameter. The experiment [4] gives the next value of $W_{\min} = (8 \pm 2.6)$ meV, that corresponds to minimum values of FWHM obtained in this model.

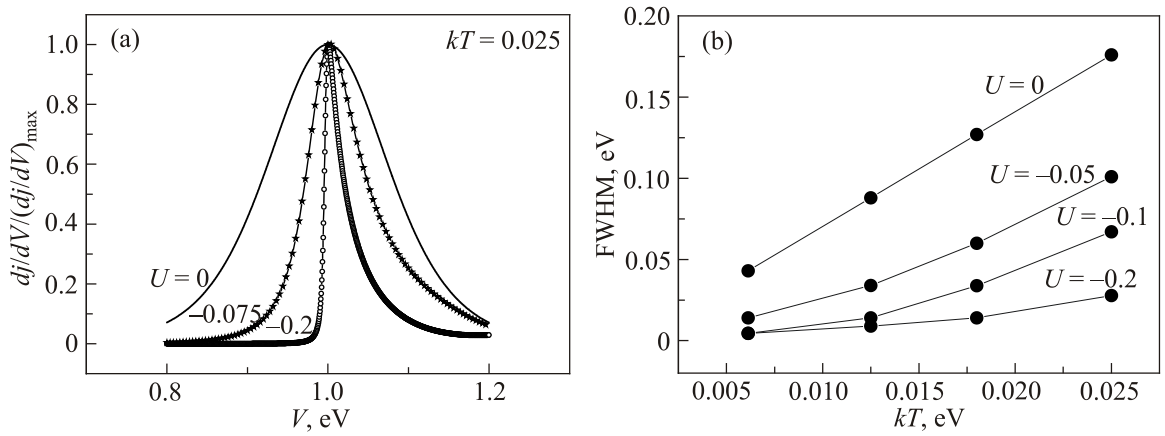

Fig. 6. Demonstration of the influence of the splitting energy U of a degenerate state in QD on FWHMs. (a) Profiles of differential conductivity normalized to maximum values and combined at maxima for different values of U = 0; –0.075; –0.2 eV and calculated at temperature kT = 0.025 eV. (b) Thermal dependences of the width of the differential conductivity peak for different values of U = 0; –0.05; –0.1; –0.2 eV.

Using the approximation $|U|/kT \gg 1$, an analytical expression can be derived for the current and its derivative. Within this approximation the next relations are valid: $f_R(E_m) = 0$ and $f_L(E_0) = 0$, and also $f_L(E_2) = f_L(E_3) = 1$. Then Eq. (5) will have the stable solution for the occupation number n

$$n = \begin{cases} 0, & \text{if} \quad f_L(E_1) < 2/3 \\ \dfrac{2(3f_L(E_1)-2)}{3(2f_L(E_1)-1)+\sqrt{12f_L(E_1)-7}}, & \text{if} \quad f_L(E_1) > 2/3 \end{cases}. \tag{10}$$

Using Eq. (10), we obtain for the current derivative

$$\frac{dJ}{dV} = J_V \begin{cases} 0, & \text{if} \quad f_L(E_1) < 2/3 \\ \dfrac{f_L(E_1)(1-f_L(E_1))}{[3(2f_L(E_1)-1)+\sqrt{12f_L(E_1)-7}]\sqrt{12f_L(E_1)-7}}, & \text{if} \quad f_L(E_1) > 2/3' \end{cases} \tag{11}$$

where $J_V = 6\gamma J_0/kT$.

In Fig. 7(a), dependences of $dj/dV = (dJ/dV)(1/J_V)$ on the applied bias V at different temperatures obtained in the approach of (10) (solid curve) and by numerical solution of Eq. (3) are shown. As can be seen in Fig. 7(a), there is a good agreement between the analytical and numerical calculation. The bias, at which a current step appears, can be found from the condition $f_L(E_1) > 2/3$. Thus, for the threshold voltage V_{th} we get

$$V_{\text{th}} = (E_g - \mu + U + kT\ln 2)/\gamma. \tag{12}$$

For the known value of V_{th}, the relation (12) may be considered as the equation for the estimation of the splitting energy value $U \approx -(E_g - \mu - \gamma V_{\text{th}})$, where it is assumed that $|U| \gg kT$. For the QD of the size L = 7 nm as was used in the experiment [4], the threshold value equals $V_{\text{th}} \approx 1$ eV, therefore, we obtain U = –0.5 eV. For the case L = 5.5 nm, the experiment [4] gives $V_{\text{th}} \approx 1.3$ eV, from that the value of U = –0.35 eV follows. In Fig. 7(b), the comparison of experimental and calculated temperature dependences of FWHMs is given. A good agreement of experimental data [4] and theory can be observed. All parameters required for calculations were defined from experimental data. From the formula (11), it also follows that the position of a current step as a function of the applied bias also depends linearly on temperature.

7. Discussion and concluding remarks

Some of the assumptions of our approach to the problem of suppressing the temperature smearing may be debatable. In particular, it concerns the role of the spatial quantization. The proposed by the authors of Ref. 4 treatment of the current steps occurrence due to the Coulomb blockade by some reasons is not a perfect one. The main drawback is that the description of the Coulomb blockade

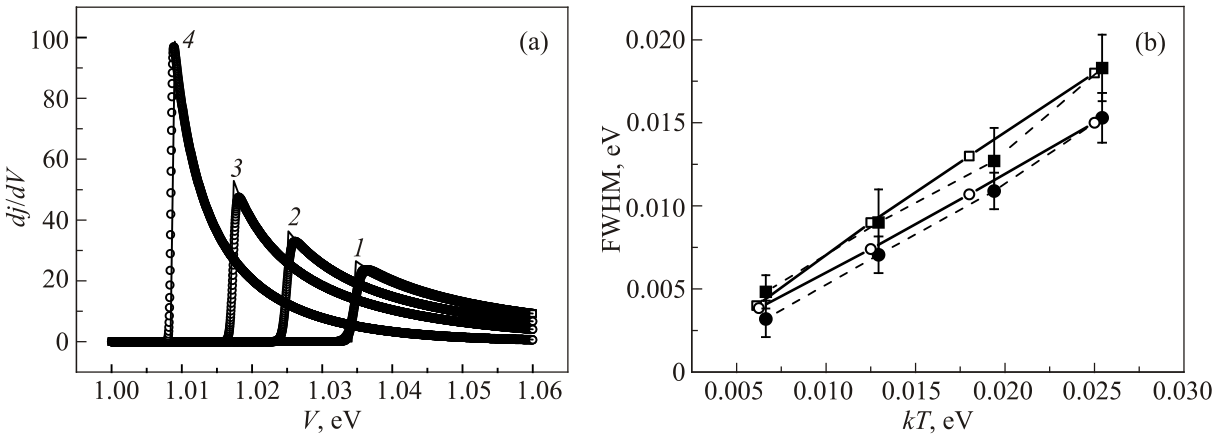

Fig. 7. (a) Differential conductivity peak as a function of bias voltage. Solid lines show dependences obtained from Eq. (10), points ○ are obtained by numerical calculation of Eq. (3) with ΔE = 0.85 eV, U = – 0.35 eV, γ = 0.5, and kT = 0.00625, 0.0125, 0.018, 0.025 eV for the curves *1*; *2*; *3*; *4*, correspondingly. (b) The width of current steps as a function of temperature, points ● are experimental values of FWHMs, obtained in Ref. 4 (dashed line) for the QD of size 7 nm, ■ — of size 5.5 nm; ○,□ — values of FWHWs obtained by numerical calculation of Eq. (3) (solid line) with the parameters values: γ = 0.5, ΔE = 1 eV, U = – 0.5 eV and – 0.35 eV, respectively.

is based on a semiclassical theory while to describe the phenomenon of the "filtration" a rigorous quantum mechanical method is needed. Thus we cannot use a classical conception of capacitance. On the other hand, the occurrence of the current steps as follows from a quantum mechanical approach may be the result of a degenerate level splitting due to Coulomb repulsion. But the estimated value of energy splitting by this mechanism is much less than the observed in the experiment.

We can argue that the Coulomb blockade takes place only in systems for which the conditions for the spatial quantization are fulfilled. This allows us to suggest that the spatial quantization is a more fundamental effect than the Coulomb blockade. Such a conclusion is confirmed by the inversely proportional relationship of the separation between steps on the dimensions of the QD (see [9]) what is also followed from Eqs. (1), (2). On the other hand, the linear dependence of the capacitance on the QD size also leads to the inverse proportional dependence of the steps separation on its size that allows treating steps as a result of changing of the QD electrostatic energy. With this approach, there is a necessity of assuming the integrity of the electron localization in the QD. In quantum mechanics, this statement is absent. Moreover, there is a fractional part of an electron in the QD because the electron wave function belongs to the whole conducting system. Therefore, in the confined space an electron may be localized only partially. Only in the case when the system becomes unconducting, the whole localization is possible.

In the experiment [4], a significantly large separation between conductivity peaks was observed. That indicates the presence of a strong electron–phonon interaction. The nature of appearance of such a large interaction is not entirely clear. In our case, estimations show that the Coulomb component in U has the value of the order of tens meV. Therefore, we can neglect the Coulomb component. In Ref. 9, the following relation for $U_{\rm ph}$ is given

$$U_{\rm ph} = \sum_i \frac{|\varphi_i|^2}{\hbar\omega_i}, \qquad (13)$$

where φ_i is a matrix element of the interaction of an electron with a phonon mode i characterized by the frequency ω_i. As follows from the relation (13), $U_{\rm ph}$ takes a large value when phonon oscillation frequencies are small, and there are a large number of them. The low energy of oscillations means that oscillating atoms are weakly bound. Such a situation is possible in principle at the surface of a nanoparticle. In this case, it is necessary to carry out the summation over vibration modes of weakly bound atoms, the number of which is proportional to the surface of the nanoparticle, i.e., L^2. On the other hand, for a nanoparticle of a small size due to changes in the surface curvature the binding abilities of atoms are broken near the surface. This will take place in the case when the shape of the particle is not a spherical one. As a result, these atoms either become strongly bound with the particle or loose the contact with it. In other words, there exists a minimum value of the particle diameter $L_{\rm min}$, at which a strong electron–phonon interaction is possible. In the standard theory of electron–phonon interaction, the matrix element φ_i depends on the particle size as $L^{-3/2}$. Thus, we obtain

$$U_{\rm ph} = P\,\frac{L^2 - L_{\rm min}^2}{L^3}, \quad \text{where} \quad L > L_{\rm min}. \qquad (14)$$

Here P is the coefficient weakly dependent on a nanoparticle size. According to the relation (13), $|U|$ takes the minimum value when $L = L_{\rm op} = \sqrt{3}L_{\rm min}$, as is illustrated in Fig. 8(a). If we suppose that in experiments of Ref. 4, the optimal nanoparticle diameter, at which the filtration effect is the most pronounced one, corresponds to the value $L_{\rm op}$ = = 7 nm. At the same time, when $|U_{\rm ph}|$ takes the maximum value, we obtain $L_{\rm min} \approx 4$ nm. So, the large size of a nanoparticle indicates that we deal with oscillations of atoms localized at the intersection of crystal faces with the surface of the particle. Evidently, in this case the value of $L_{\rm min}$ depends on the method of preparing of nanoparticles. With the particle diameter $L \approx 5.5$ nm, as follows from Fig. 8(a), the value of the splitting energy is $U \approx -0.35$ eV which approximately equals to the value used in our calculations.

The considered mechanism of suppression of thermal effects under tunneling suggests the appearance of strong asymmetry of conductivity peaks that is not observed in the experiment. One of the reasons of this, in our opinion, may be the voltage fluctuations in the system. Indeed, since the appearance of a current step has a threshold character then slight fluctuations of the voltage near the threshold can significantly change the conductivity of the tunnel system. In other words, strong fluctuations can be initiated by the external bias. The account of the fluctuation effect on the conductivity may be carried out by the addition of the term $\beta(0,5 - R)$ to the energy E_m, where R in the interval of $0 \le R \le 1$ takes a random value, and β defines the amplitude of fluctuations. In Fig. 8(b), dependences of the current step profile and the current derivative on the bias with an account of random voltage fluctuations are shown.

Negligible (few fractions of a percent) fluctuations of voltage can lead to significant fluctuations of the current derivative. Therefore, in this case the derivative was calculated by the smoothing method. As can be seen in the figure, the shape of the derivative with account of fluctuations becomes more symmetrical and takes triangular form observed in the experiments.

It is worth to note that an attractive interaction leading to electron–electron pairing is not a unique phenomenon in nanoobjects. For example, in Refs. 15, 16 it was reported about the experiments on nanowires that demonstrate the existence of electron pairing without superconductivity.

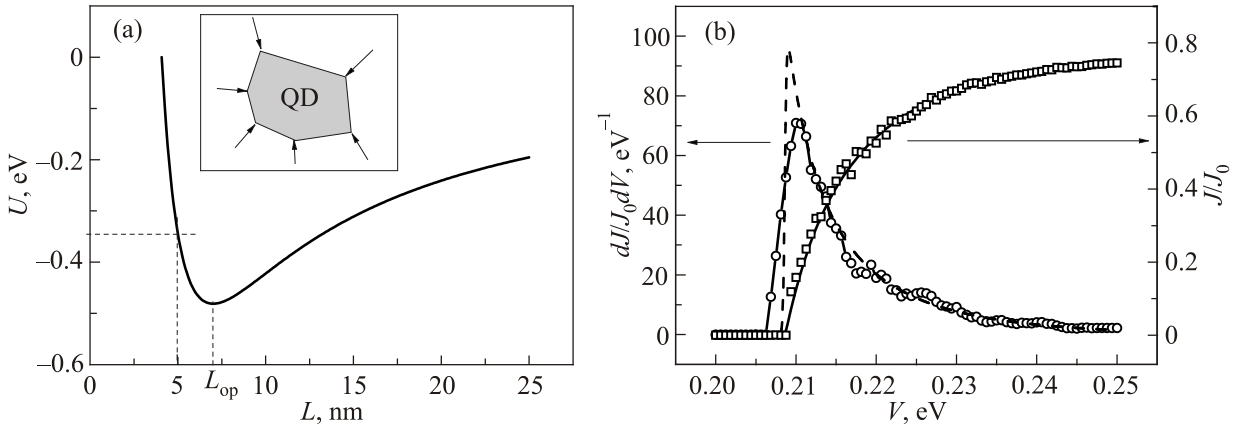

Fig. 8. (a) The splitting energy U dependence (solid curve) on the QD size obtained from the relation (13), where P = 5 eV·nm. The inset shows a schematic section through a nanoparticle. Arrows point to the intersections of the crystal faces that come out on the surface on which weakly bound atoms may be localized. (b) Profile of the current step (□) and derivative of a current (○) functions on the bias voltage V with account of random oscillations of the voltage for U = 0.1 eV, ΔE = 0.1 eV, κT = 0.00625 eV. (○ points were obtained by means of smoothing of the derivative.) Amplitude coefficient of random fluctuations has the value β = 0.0015 eV.

We have shown that the effect of suppressing the thermal distribution of current carriers can be explained by the model of resonant tunneling with nonlinearity caused by the strong electron–phonon interaction leading to the attractive interactions of electrons. We can also assume that in this model the presence of Fano resonance can be found, that is connected with a many channel tunneling, but since the phenomenon has a threshold character, then the Fano resonance is smeared. In the proposed description of the effect of cold electrons filtering, fitting parameters are absent, and nevertheless a good agreement between theory and experiment has been achieved.

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Нелінійне резонансне тунелювання як механізм фільтрації холодних електронів

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Стаття присвячується поясненню ефекту придушення температурного розподілу носіїв струму в тунельному пристрої, де наночастинка, впроваджена в діелектричну матрицю, виконує роль квантової точки (КТ). Через просторове обмеження в КТ має місце квантування енергії. Припускається, що кожний рівень чотирьохкратно вироджен. Ми вважаємо наявність в КТ сильної електрон-фононної взаємодії, що призводить до взаємодії між електронами, яка перевищує

кулонівське відштовхування. У результаті такої взаємодії виродження рівнів знімається. Дискретні енергетичні рівні можуть мати енергії менше, ніж енергія Фермі в електроді. Тунельний струм через ці рівні не буде залежати від температури. Незважаючи на те, що в запропонованому механізмі фільтрації холодних електронів відсутні підгінні параметри, досягнуто добре узгодження теорії з експериментом.

Ключові слова: резонансне тунелювання, квантова точка, фононна взаємодія, фільтрація енергії електронів.

Нелинейное резонансное туннелирование как механизм фильтрации холодных электронов

В.Н. Ермаков, Е.А. Понежа

Статья посвящается объяснению эффекта подавления температурного распределения носителей тока в туннельном устройстве, где наночастица, внедренная в диэлектрическую матрицу, выполняет роль квантовой точки (КТ). Через пространственное ограничение в КТ будет иметь место квантование энергии. Предполагается, что каждый уровень четырехкратно вырожден. Мы предполагаем наличие в КТ сильного электрон-фононного взаимодействия, что приводит к притяжению между электронами, превышающему кулоновское отталкивание. В результате такого взаимодействия вырождение уровней снимается. Дискретные энергетические уровни могут иметь энергии, меньшие энергии Ферми в электроде. Туннельный ток через эти уровни не будет зависеть от температуры. Несмотря на то, что в предлагаемом механизме фильтрации холодных электронов отсутствуют подгоночные параметры, достигнуто хорошее согласие теории с экспериментом.

Ключевые слова: резонансное туннелирование, квантовая точка, электрон-фононное взаимодействие, фильтрация энергии электронов.