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ELECTRON TUNNELING IN THE GERMANIUM/SILICON HETEROSTRUCTURE WITH GERMANIUM QUANTUM DOTS: THEORY

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It is shown that electron tunneling through a potential barrier that separates two quantum dots of germanium leads to the splitting of electron states localized over spherical interfaces (a quantum dot – a silicon matrix). The dependence of the splitting values of the electron levels on the parameters of the nanosystem (the radius a quantum dot germanium, as well as the distance D between the surfaces of the quantum dots) is obtained. It has been shown that the splitting of electron levels in the QD chain of germanium causes the appearance of a zone of localized electron states, which is located in the bandgap of silicon matrix. It has been found that the motion of a charge-transport exciton along a chain of quantum dots of germanium causes an increase in photoconductivity in the nanosystem.

It is shown that in the QD chain of germanium a zone of localized electron states arises, which is located in the bandgap of the silicon matrix. Such a zone of local electron states is caused by the splitting of electron levels in the QD chain of germanium. Moreover, the motion of an electron in the zone of localized electron states causes an increase in photoconductivity in the nanosystem. The effect of increasing photoconductivity can make a significant contribution in the process of converting the energy of the optical range in photosynthesizing nanosystems. It has been found that comparison of the splitting dependence of the exciton level $E_{ex}(a)$ at a certain radius a QD with the experimental value of the width of the zone of localized electron states arising in the QD chain of germanium, allows us to obtain the distances D between the QD surfaces.

It has been shown that by changing the parameters of Ge/Si heterostructures with germanium QDs (radius of a germanium QD, as well as the distance D between the surfaces of the QDs), it is possible to vary the positions and widths of the zones of localized electronic states. The latter circumstance opens up new possibilities in the use of such nanoheterostructures as new structural materials for the creation of new nano-optoelectronics and nano-photosynthesizing devices of the infrared range.

Keywords: splitting of electronic states, charge-transfer exciton, spherical interface, potential barrier, Coulomb interaction, quantum dots

INTRODUCTION

In Ge/Si heterostructures with germanium quantum dots (QDs) are of the second type, the main electron level was in the silicon matrix, and the main level of holes was in the germanium QD [1-8]. A significant shift of the shift of the valence band ($\Delta E_{\nu(Ge)} = 610$ meV) of germanium QDs (relative to the ceiling of the valence band of the silicon matrix) caused hole localization in the ODs. A substantional shift of the bottom of the conduction band ($\Delta E_{c(Si)} = 340 \text{ meV}$) of the silicon matrix (relative to the bottom of the conduction band of germanium QDs) in the heterostructure was a potential barrier for electrons (electrons moved in the matrix and did not penetrate into the QD) [1-8]. When studying the optical properties of Ge/Si nanoheterostructures with germanium QDs, experimental work [1] was the first to reveal the spatial separation of electrons and holes, as a result of which electrons were localized above the QD surface, and holes moved into QDs. The transition between such states was indirect in space [1, 2, 9]. In experimental studies [1, 2] it was found that in nanosystems consisting of germanium QDs located in silicon matrices, the excitation of spatially indirect excitons (SIE) is possible [3–8].

The effect of significant increase in the SIE binding energy (by almost two orders of magnitude) is found in nanosystems containing semiconductor (cadmium sulfide, zinc selenide, germanium) QDs, compared with the exciton binding energy in the corresponding single crystals [3–5]. Such an effect of significant increase in the SIE binding energy opens a possibility for the use of nanosystems as an active field of nanolasers operating on exciton transitions at room temperature.

In [9], heterostructures, which are linear germanium QD chains on silicon substrates, were obtained using the method of electron beam lithography. The average radii of QD of germanium did not exceed 30 nm. In Ge/Si heterostructures with germanium QDs, it was found in experimental works [1, 2] that lowtemperature optical absorption and photoluminescence spectra were caused by interband electron transitions from the valence band of germanium QD to the conduction band of the silicon matrix. The photoluminescence signal of nanostructures in the infrared spectral region 0.20-1.14 eV was observed up to room temperature [1–8].

At low concentrations N QDs of germanium, when in linear chains the average distance (~ $N^{-1/3}$) between the surfaces of the QD significantly exceeds the Bohr radius of the electron $a_e = 0.63$ nm in the silicon matrix, that is,

$$a_e N^{1/3} << 1$$
, (1)

the interaction between QDs can be neglected. The optical properties of such nanosystems were mainly determined by the energy spectra of electrons and holes localized near the surface of single germanium QDs grown in a silicon matrix [1-5, 7, 8].

With the increase of the concentration N of germanium QD in linear chains the average distance between the surfaces of the QD decreased. In nanostructures with large concentrations N of QDs at distances between the QD surfaces (about a_e), it is necessary to take into account the interaction between the QD surfaces. In this case, the condition should be satisfied

$$a_e N^{1/3} \sim 1$$
 . (2)

As the spacing between the QDs surfaces is decreased, the overlapping integral S(a, D) of the exciton wavefunctions and the energy of the exchange interaction of the electrons with the holes substantially increase. Therefore, a coupled state of two excitons formed in the nanosystem; *i.e.*, an exciton quasimolecule consisting of two QDs appeared in the nanosystem [6]. In such exciton quasimolecule, electrons and holes were separated in space (the holes moved in germanium QDs, and the electrons were localized over a spherical interface (QD – silicon matrix)). In [6], it was shown that the appearance of a quasimolecule had a threshold nature and was

possible in the nanosystem, in which the distance D between the surfaces of the QDs was determined by the condition $D_c^{(1)} \le D \le D_c^{(2)}$. The existence of such a distance $D_c^{(1)}$ was due to quantum size effects, in which the decrease in the energies of interaction of the electrons and holes entering into the Hamiltonian of the exciton quasimolecule with decrease of the distance D between the QD surfaces could not compensate for the increase in the kinetic energy of electrons and holes. At larger distance D between the surfaces of QDs, such that $D \ge D_c^{(2)}$, the exciton quasimolecule splits into two excitons (from spatially separated electrons and holes).

At present, the optical properties of Ge/Si heterostructures with germanium QDs have not yet been adequately studied. In particular, there are no works that investigate electron tunneling between the surfaces of germanium QDs on silicon substrates. Therefore, in this paper, in contrast to [3, 5], the splitting of electron states localized over a spherical interface (germanium QD – silicon matrix) due to electron tunneling through a potential barrier separating two QDs is investigated.

THE SPLITTING OF ELECTRON STATES IN Ge/Si HETEROSTRUCTURE WITH QUANTUM DOTS

In [6], a model of nanosystems consisting of two spherical QD(A) and QD(B) with radius a, containing germanium with a dielectric constant $(\varepsilon_2 = 16.3)$ grown in a silicon matrix with a dielectric constant ($\varepsilon_1 = 11.7$). It was assumed that the holes h(A) and h(B) with effective masses $((m_{\rm h}/m_0) = 0.39)$, were located at the centers of QD(A) and QD(B). In the nanosystem, electrons e(1) and e(2)with effective masses $((m_e^{(1)}/m_0) = 0.98)$ were localized over the spherical surfaces of QD(A) and QD(B) in potential wells caused by the Coulomb attraction $V_{\rm eh}(x)$ electron and hole in a silicon matrix. The energy of the Coulomb interaction of an electron with a hole was described by the formula [3]

$$V_{eh}(x) = -\frac{e^2}{\tilde{\varepsilon}x}$$
(3)

(where $\tilde{\varepsilon} = 2\varepsilon_1\varepsilon_2/(\varepsilon_1 + \varepsilon_2)$ – dielectric constant of the nanosystem, x – electron distance from the surface of the QD). If in the nanosystem with a

high concentration of QDs N (condition (2) is satisfied), the distance D between the surfaces of the germanium QDs exceeded the value $D_c^{(2)}$, then the exciton quasimolecule would have been decayed into two excitons in which electrons were located above the spherical interface (QD – matrix), and the holes were in the valence band of germanium QDs [6].

If the distances D between the surfaces of QD of germanium in the nanosystem exceeded the value of $D_c^{(2)}$, then the exciton quasimolecule decayed into two excitons, in which electrons were localized above the spherical interface (QD - matrix), and the holes were in the valence band of germanium QD [6]. Such excitons appeared when the photon with the energy smaller than the width of the band gap $E_{g(Si)}$ of the silicon matrix was absorbed by the nanosystem [7]. The ground state $E_0(a)$ of the exciton with the increase of the radius QD *a* (so that $a \ge 22.2$ nm) passed into the ground state of a two-dimensional exciton (from a spatially separated electron and hole) localized above the flat interface (germanium – silicon) with the energy [3]

$$E_0(a) = -E_{ex}^{2D}, \quad E_{ex}^{2D} = 2\hbar^2 / \mu_{ex}^{2D} \left(a_{ex}^{2D} \right)^2, \tag{4}$$

where $E_{ex}^{2D} = 82 \text{ meV} - \text{is the binding energy of}$ the two-dimensional SIE. The Bohr radius of such SIE is

$$a_{ex}^{2D} = \tilde{\varepsilon} \left(m_0 / \mu_{ex}^{2D} \right) \left(2\hbar^2 / m_0 e^2 \right),$$
 (5)

where $\mu_{ex}^{2D} = m_e^{(1)} m_h / (m_e^{(1)} + m_h)$ – the reduced mass of the SIE, wherein $a_{ex}^{2D} = 2.6$ nm.

In [3] and [6], the energy of the SIE state $E_0(a)$ was measured from the bottom of the conduction band of the silicon matrix ($E_{c(Si)} = E_{g(Si)} = 1.17 \text{ eV}$). Between the electronic states localized over the spherical surfaces of QD(A) and QD(B), tunneling is possible through the potential barrier that separates these QDs. Such a potential barrier is caused by the Coulomb attraction $V_{eh}(x)$ (3) of electrons e(1) and e(2) to their holes located in the centers of QD(A) and QD(B) (see Fig. 1). We can write the expression describing the potential barrier U(x) in this form:

$$U(x) = -\frac{e^2}{\tilde{\varepsilon}((D/2) - x)}, \quad 0 \le x \le (D/2), \tag{6}$$

$$U(x) = -\frac{e^2}{\tilde{\varepsilon}((D/2) + x)}, \quad (-D/2) \le x \le 0.$$
(7)

The potential energy U(x) consists of two symmetric potential wells (6) and (7), separated by a potential barrier of height

$$U_0(D) = U(x=0) = -\frac{2e^2}{\tilde{\varepsilon}D}.$$
 (8)

Electron tunneling through the potential barrier U(x) (6)–(8), separating two QDs causes the splitting of the exciton energy level $E_{ex}(a)$, which is located in the potential wells U(x) (6), (7) in the silicon matrix at two close exciton levels $E_{ex}^{(1)}(a)$ and $E_{ex}^{(2)}(a)$. Such close exciton levels $E_{ex}^{(1)}(a)$ and $E_{ex}^{(2)}(a)$ correspond to states in which the electron moves simultaneously in both potential wells U(x) (6), (7). We will assume that the potential barrier U(x) (6), (7) is described by a semiclassical field. Using approach [10], we obtain the expression that determines the splitting $\Delta E_{ex}(a, D) = (E_{ex}^{(1)}(a) - E_{ex}^{(2)}(a))$ of the exciton level $(E_{ex}(a) = -E_0(a) = E_0)$

$$\Delta E_{ex}(a,D) = \left(\hbar\omega_0(a,D)/\pi\right) \exp\left[-\left(2/\hbar\right)\int_0^b p(x)dx\right].$$
(9)

In formula (9), the quantity

$$\omega_0(a,D) = \left(\pi/\mu_{ex}^{2D}\right) \left[\int_0^b dx/p(x)\right]^{-1}$$
(10)

describes the frequency of the classical periodic electron motion in the field U(x) (6), (7), p(x)determines the momentum of an electron moving in the field U(x) (6), (7), wherein

$$p(x) = \left[-2\mu_{ex}^{2D} \left(U(x) + E_0\right)\right]^{1/2},$$
(11)

b – turning point whose value is determined from the expression $U(x = b) = E_0(a)$.

After integrating formula (9), taking into account (6)–(8), we obtain an expression that describes the splitting $\Delta E_{ex}(a, D)$ of the exciton level ($E_{ex}(a) = -E_0$)

$$\Delta E_{ex}(a,D) = 2^{-3/2} \left\{ \left[1 - \left(\tilde{E}_0 \tilde{D} \right)^{1/2} \left(\tilde{E}_0 \tilde{D} - 1 \right)^{1/2} \right] \left(2\tilde{E}_0 \right)^{-3/2} + \left(1 + \ln \left[\left(\tilde{E}_0 \tilde{D} \right)^{1/2} + \left(\tilde{E}_0 \tilde{D} - 1 \right)^{1/2} \right] \right\}^{-1} \cdot \right\}$$

$$\cdot \left[\left(\tilde{E}_0 \tilde{D} \right)^{1/2} + \left(\tilde{E}_0 \tilde{D} - 1 \right)^{1/2} \right]^{-2\sqrt{2}} \exp \left[-2 \tilde{D}^{1/2} \left(\tilde{E}_0 \tilde{D} - 1 \right)^{1/2} \right] E_{ex}^{2D},$$
(12)

where $(\widetilde{E_0} = (E_0/E_{ex}^{2D}))$ and $\widetilde{D} = (D/a_{ex}^{2D})$. Formula (12) is valid only for the weak splitting $\Delta E_{ex}(a, D)$ of the exciton level $\Delta E_{ex}(a)$. In this case, the following condition should be satisfied

$$(\Delta E_{ex}(a,D)/E_0) \ll 1 \tag{13}$$

Expression (12) is obtained in the semiclassical approximation, in which it is assumed that the potential field U(x) (6), (7) is a semiclassical field. In this case, the condition [10] should be satisfied

$$\hbar d/(dx)(p(x))^{-1} << 1 \tag{14}$$

which is performed at

$$\left(\tilde{E}_0\tilde{D}\right) > 1. \tag{15}$$

Magnitude splitting (12) is $\Delta E_{ex}(a, D) > 0$, if

$$\left(\tilde{E}_{0}\tilde{D}\right)^{1/2}\left(\tilde{E}_{0}\tilde{D}-1\right)^{1/2}<1.$$
(16)

Conditions (15) and (16) are satisfied when

$$\left(\tilde{E}_0\tilde{D}\right)^{1/2} > 2^{-1}\left(1+5^{1/2}\right).$$
 (17)

Thus, the fulfillment of the requirement (17)allows us to obtain an expression that describes the splitting $\Delta E_{ex}(a, D)$ (12) of the exciton level $E_{ex}(a)$, in the semiclassical approximation. From formula (12) it is followed that with the increase in the distance D between the surfaces of the QD (so that $\tilde{D} >> 1$) the splitting $\Delta E_{ex}(a, D)$ decreases $(\Delta E_{ex}(a,D) \sim \tilde{D}^{-\sqrt{2}})$. Therefore, in a nanosystem with a small concentration of QDs N(so that condition (1) is satisfied), the probability of electron tunneling through the potential barrier U(x) (6)–(8) separating two QDs takes a small value. In this case, the splitting values $\Delta E_{ex}(a, D)$ (12) of the exciton levels $E_{ex}(a)$ will be negligible compared with the energies of the excitonic levels $E_{ex}(a)$.

The exciton levels $E_0(a)$ as well as the potential barrier U(x) (6)–(8) are in the forbidden zone of the silicon matrix. Therefore, in order for the potential barrier U(x) (6)–(8) to be located in

the forbidden zone of the silicon matrix, a condition is true:

$$|U_0(D)| < E_{g(Si)}.$$
 (18)

Requirement (18), taking into account (8), (4) and (5), is satisfied for nanosystems in which the distance D between the surfaces of the QDs exceeds the value

$$D > \left(E_{ex}^{2D} / E_{g(Si)} \right) a_{ex}^{2D}.$$
 (19)

Inequality (19) holds for nanosystems in which the distances D between the surfaces of the QDs exceed the values (D > 0.18 nm).

The positions of the exciton levels $E_0(a)$, which are located in the band gap of the silicon matrix, do not depend on the temperature *T*, if the distances of these levels from the bottom of the conduction band $E_{c(Si)}$ of the silicon matrix significantly exceed the thermal energy (k_BT) of the electron (where k_B is a constant Boltzmann), i.e. the following condition must be met

$$\left(E_{c(Si)} + E_0(\alpha)\right) >> k_B T.$$
⁽²⁰⁾

RESULTS AND DISCUSSION

We will estimate the splitting $\Delta E_{ex}(a, D)$ (12) of the exciton levels $(E_{ex}(\bar{a}_1) = -E_0(\bar{a}_1) = -64 \text{ meV}$ $(E_{ex}(\overline{a}_2) = -E_0(\overline{a}_2) = -72 \text{ meV})$ and in the nanosystem consisting of a chain of germanium QDs with average radii $\overline{a}_1 = 12.8 \ nm$ and $\overline{a}_{2} = 15 \text{ nm}$, grown in a silicon matrix, and studied under experimental conditions [9] (see Table 1 and Table 2). For average distances D between the surfaces of QDs, which continuously vary in the range from $D_1 = 7.8$ nm to $D_2 = 8.4$ nm, using the formula (12), we obtain for the exciton level $E_{ar}(\overline{a}_1)$ the splitting values $\Delta E_{ex}(a, a)$ D) monotonically varying in the interval from $\Delta E_{ex}(\overline{a}_1, D_1) = 8 \ meV$ to $\Delta E_{ex}(\overline{a}_1, D_2) = 0.16 \ meV$ (see Table 1). In this case, for the exciton level $E_{ex}(\overline{a}_2)$ the splitting $\Delta E_{ex}(a, D)$ takes a monotonically varying value in the range from $\Delta E_{ex}(\overline{a}_2, D_1) = 8.8 \text{ meV}$ to $\Delta E_{ex}(\overline{a}_2, D_2) = 0.2 \text{ meV}$ (see Table 2). Such splittings $\Delta E_{ex}(\overline{a}_1, D_1)$ and $\Delta E_{ex}(\overline{a}_1, D_2)$ correspond to the temperatures and $T_2^{(1)} = 1.85 K$. Splittings $\Delta E_{ex}(\overline{a}_2, D_1)$ and $\Delta E_{ar}(\overline{a}_{2}, D_{2})$ correspond to the temperatures $T_1^{(2)} = 102 K$ and $T_2^{(2)} = 2.3 K$. Requirements (13)

for the smallness of splitings $\Delta E_{ex}(\overline{a}_1, D)$ and $\Delta E_{ex}(\overline{a}_2, D)$ in comparison with the value of the

energy of the exciton levels $E_0(\overline{a}_1)$ and $E_0(\overline{a}_2)$ are satisfied.

Table 1. Dependence of the splitting $\Delta E_{ex}(\overline{a_1}, D)$ (12) of the exciton level $(E_0(\overline{a_1}) - 64 \text{ meV})$ in a nanosystem that consists of two germanium QDs with average radii $\overline{a_1} = 12.8 \text{ nm}$, on the distance D between the surfaces of the QD

\bar{a}_1 , nm	$E_0(\bar{a}_1)$, meV	D, nm	$\Delta E_{ex}(\bar{a}_{1},\mathbf{D}), \text{meV}$
2.8	64	7.8	8
2.8	64	8	2.4
2.8	64	8.2	0.64
2.8	64	8.4	0.16

The splitting values $\Delta E_{ex}(\overline{a}_1, D)$ and $\Delta E_{ex}(\overline{a}_2, D)$, according to (12), have a strong exponential dependence on the distance D between the surfaces QD. With a slight increase in the distance D from $D_1 = 7.8$ nm to $D_2 = 8.4$ nm, the splitting values $\Delta E_{ex}(a, D)$ (12) substantially decrease from $\Delta E_{ex}(\overline{a}_1, D_1) = 8$ meV to $\Delta E_{ex}(\overline{a}_1, D_2) = 0.16 \text{ meV}$, as well as from $\Delta E_{ex}(\overline{a}_2, D_1) = 8.8 \text{ meV}$ to $\Delta E_{ex}(\overline{a}_2, D_2) = 0.2 \text{ meV}$ (see Table 1 and Table 2). With an increase in the

average radius of the QD a (from $\overline{a}_1 = 12.8 \ nm$ to $\overline{a}_2 = 15 \ nm$), the exciton level energy values $E_0(a)$ increase (from $E_0(\overline{a}_1) = 64 \ meV$ to $E_0(\overline{a}_2) = 72 \ meV$ [3].

It should be noted that the estimates of the splitting values $\Delta E_{ex}(a, D)$ (12) of the exciton levels $E_{ex}(a)$ are obtained here within the framework of the theory we have developed, and the conditions (13), (14) and (18)–(20) are satisfied.

Table 2. Dependence of the splitting $\Delta E_{ex}(\overline{a}_2, D)$ (12) of the exciton level $(E_0(\overline{a}_2) = -72 \text{ meV})$ in a nanosystem that consists of two germanium QDs with average radii $\overline{a}^2 = 15nm$, on the distance D between the surfaces of the QD

<i>ā</i> 2, nm	$E_0(\bar{a}_2)$, meV	D, nm	$\Delta E_{ex}(\bar{a}_{2},\mathbf{D}), \mathbf{meV}$
5	72	7.8	8.8
5	72	8	2.8
5	72	8.2	0.78
5	72	8.4	0.2

It was shown in [3] that in a Ge/Si nanosystem with germanium QDs in the interval of average QD radii (6.4 nm $\le a \le 22.2$ nm) upon absorption of a quantum of light with energy

$$\hbar \omega_{ex}(a) = E_{g(Ge)} - \Delta E_{c(Si)} - E_{ex}(a), \qquad (21)$$

in the band gap of the silicon matrix, an SIE state with energy $E_{ex}(a)$ appeared. In formula (21), $E_{ex}(a)$ is the SIE binding energy, and the value $\left(E_{g(Ge)} - \Delta E_{g(Si)}\right) = 330 \text{ meV}$. For the appearance in the nanosystem with germanium QDs with radii $\overline{a}_1 = 12.8 \text{ nm}$ and $\overline{a}_2 = 15 \text{ nm}$ of exciton levels $\left(E_{ex}(\overline{a}_1) = -64 \text{ meV}\right)$ and $\left(E_{ex}(\overline{a}_2) = -72 \text{ meV}\right)$, according to (21), light quanta with following energies $\hbar \omega_{ex}(\bar{a}_1) = 266 \text{ meV}$ and $\hbar \omega_{ex}(\bar{a}_2) = 258 \text{ meV}$ are required. Such energies $\hbar \omega_{ex}(\bar{a}_1) = 266 \text{ meV}$ and $\hbar \omega_{ex}(\bar{a}_2) = 258 \text{ meV}$ were contained in the infrared spectral region 0.20–1.14 eV, which was observed under experimental conditions up to room temperature [1, 2].

Let us assume that the distances D between the surfaces of the QDs will be the same in the entire linear chain of germanium QDs on the substrate of the silicon matrix [9]. As a result of electron tunneling through the potential barrier U(x) (6)–(8), which separates QDs, the exciton states $E_{ex}(a)$ are splitted, forming a zone of localized electron states in a linear germanium QD chain. The qualitative estimate of the width of the zone of localized electronic states gives a value that is determined by the magnitude of the order of splitting $\Delta E_{ex}(a, D)$ (12) of the exciton levels $E_{ex}(a)$. Such a zone of localized electronic states is located in the band gap of the silicon matrix. The position of the zone of localized electron states in the nanosystem is determined by the position of the exciton level $E_0(a)$. With an increase in the average radius of QD a (for $a \ge 22.2$ nm), the exciton level $E_0(a)$ approached the ground level of the two-dimensional exciton $E_{ex}^{2D} = 82 \text{ meV}$ (4) [3]. The position of the zone of localized electron states also approaches the main level of the two-dimensional SIE E_{er}^{2D} (4) (see Fig.). Thus, the position of the zone of localized electronic states depends on the average radius a of the QD, and the width of the zone of localized electronic states depends on the distance D between the surfaces of the QD. Comparing the splitting dependence $\Delta E_{ex}(a, D)$ (12) of the exciton level $E_{ex}(a)$ at a certain QD's radius a with the experimental value of the width of the zone of localized electron states arising in the QD chain of germanium, one can obtain the distances D between the QD surfaces.



Fig. The schematic plot of potential barrier U(x) (6)–(8), which separates two QD, the heigh $U_0(D)$ (8) of potential barrier, exciton level position $E_0(a)$, radius *a* of QD, distance *D* between the surfaces of QD of germanium

In the linear chain of germanium QDs [9], due to translational symmetry, the electronic excitation moves in the zone of localized electron states. In this case, the electron excitation in the nanosystem is a charge-transfer exciton [11], in which the hole is in the valence band of a germanium QD, and the electron, tunneling between the quantum dots, moves in the zone of localized electron states. As the QD radius a increase, the binding energy $|E_{ex}(a)|$ of the ground state of the exciton in the nanosystem increased [3]. Therefore, the distance D, for which the square of the overlapping integral S(D, a) of the exciton wave functions took the maximum value, decreased with increasing radius QD a [6]. The spatial separation of electrons and holes in a Ge/Si heterostructure with germanium QDs resulted in a small overlap integral of electron and hole wave functions that described the motion of electrons and holes in a nanoheterostructure not exceeding the value (≈ 0.08) [6]. Therefore, the lifetimes of excitons from spatially separated electrons and holes are substantially longer (by two orders of magnitude) to the lifetimes of excitons in a single crystal of silicon [1, 2, 9]. The motion of such a "long-lived" electron in the zone of localized electronic states located in the band gap of the matrix leads to increase silicon an in photoconductivity in the nanosystem.

Using approach [10], we obtain an expression that qualitatively describes the current density j(a, D), caused by the movement of electrons in the zone of localized electron states

$$j(a,D) \approx K(a,D) \approx \exp\left[-2\tilde{D}^{1/2} \left(\tilde{E}_0 \tilde{D} - 1\right)^{1/2}\right].$$
(22)

In formula (22) K(a, D) determines the coefficient of transparency of the potential barrier U(x) (6)–(8). With the increase of the distance D between the QD surfaces (so that $\tilde{D} >> 1$) the current density j(a, D) (22) decreases $(j(a, D) \sim exp(-\tilde{D}))$.

CONCLUSIONS

It is shown that in the QD chain of germanium, a zone of localized electron states arises, which is located in the bandgap of the silicon matrix. Such a zone of local electron states is caused by the splitting of electron levels in the QD chain of germanium. Moreover, the motion of an electron in the zone of localized electron states causes an increase in photoconductivity in the nanosystem. The effect of increasing photoconductivity can make a significant contribution in the process of converting the energy of the optical range in photosynthesizing nanosystems [10].

It has been found that comparison of the splitting dependence $\Delta E_{ex}(a, D)$ (12) of the exciton level $E_{ex}(a)$ at a certain radius *a* QD with the experimental value of the width of the zone of localized electron states arising in the QD chain of germanium, allows us to obtain the distances *D* between the QD surfaces.

It has been shown that by changing the parameters of Ge/Si heterostructures with germanium QDs (radius *a of* germanium QD, as well as the distance *D* between the surfaces of the QDs), it is possible to vary the positions and widths of the zones of localized electronic states. The latter circumstance opens up new possibilities in the use of such nanoheterostructures as new structural materials for the creation of new nano-optoelectronics and nano-photosynthesizing devices of the infrared range.

Тунелювання електронів в гетероструктурі германій/кремній з германієвими квантовими точками: теорія

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Показано, що тунелювання електронів через потенціальний бар'єр, що розділяє дві квантові точки (КТ) германію, призводить до розщеплення електронних станів, локалізованих на сферичних поверхнях поділу (квантова точка – кремнієва матриця). Отримано залежність величин розщеплення електронних рівнів від параметрів наносистеми (радіуса квантової точки германію, а також відстані D між поверхнями квантових точок). Показано, що розщеплення електронних рівнів в ланцюжку КТ германію призводить до появи зони локалізованих електронних станів, яка розташована в забороненій зоні кремнієвої матриці. Виявлено, що рух екситона з перенесенням заряду по ланцюжку квантових точок германію викликає збільшення фотопровідності в наносистемах.

Показано, що в ланцюжку КТ германію виникає зона локалізованих електронних станів, яка розташована в забороненій зоні кремнієвої матриці. Така зона локальних електронних станів обумовлена розщепленням електронних рівнів в ланцюжку КТ германію. Крім того, рух електрона в зоні локалізованих електронних станів викликає збільшення фотопровідності в наносистемах. Ефект збільшення фотопровідності може внести істотний внесок в процес перетворення енергії оптичного діапазону в фотосинтезуючих наносистемах. Встановлено, що порівняння залежності розщеплення екситонного рівня $E_{ex}(a)$ з певним радіусом КТ з експериментальним значенням ширини зони локалізованих електронних станів, що виникають в ланцюжку КТ германію, дозволяє отримати значення відстаней D між поверхнями КТ.

Показано, що, змінюючи параметри гетероструктур Ge/Si з КТ германію (радіуси КТ германію, а також відстані D між поверхнями КТ), можна змінювати положення і ширину зон локалізованих електронних станів. Остання обставина відкриває нові можливості використання таких наногетероструктур. як нових конструкційних матеріалів для створення нової нанооптоелектроніки і нано-фотосинтезуючих пристроїв інфрачервоного діапазону.

Ключові слова: розщеплення електронних станів, екситон із перенесенням заряду, сферичний інтерфейс, потенціальний бар'єр, кулонівська взаємодія, квантові точки

REFERENCES

- 1. Yakimov A.I., Dvurechensky A.V., Nikiforov A.I. Spatially Separated Excitons in Type II Heterostructures Ge/Si. *JETP Lett.* 2001. **73**(6): 529.
- Yakimov A.I., Dvurechensky A.V., Nikiforov A.I. Spatially Separated Excitons in Heterostructures Ge/Si. JETP Lett. 2001. 119(3): 529.
- 3. Pokutnyi S.I. Excitons based on spatially separated electrons and holes in Ge/Si heterostructures. *Low Temp. Phys.* 2016. **42**(12): 1151.
- 4. Pokutnyi S.I. Binding Energy of the Exciton of a Spatially Separated Electron and Hole in Quasi-Zero-Dimensional Semiconductor Nanosystems. *Tech. Phys. Lett.* 2013. **39**(3): 233.
- 5. Pokutnyi S.I. Exciton spectroscopy with spatially separated electron and hole in Ge/Si heterostructures germanium quantum dots. *Low Temp. Phys.* 2018. **44**(8): 819.
- 6. Pokutnyi S.I. Biexciton in nanoheterostructures of germanium quantum dots. Opt. Eng. 2017. 56(6): 067104.
- 7. Pokutnyi S.I. Polarizability of germanium quantum dots with spatially separated electrons and holes in Ge/Si heterostructure. *Philos. Mag. Lett.* 2019. **99**(10): 386.
- 8. Pokutnyi S.I. Polarizability of germanium quantum dots with spatially separated electrons and holes. *The European Physical Journal Plus.* 2020. **135**(1): 74.
- 9. Smagina J., Dvurechensky A.V., Seleznev V.A. Optical properties of a chain of germanium quantum dots. Semiconductors. 2015. 49(8): 749.
- 10. Landau L.D., Lifshitz E.M. Course of Theoretical Physics. In: *Quantum Mechanics*. V. 3. (New York: Pergamon Press, 1974).
- Antonyuk B.P., Antonyuk V.P., Frolov A.A. Excitons with charge transfer in nanosystems. *Opt. Commun.* 2000. 174(4): 427.

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