ISSN 1063-7826, Semiconductors, 2008, Vol. 42, No. 13, pp. 1462–1468. © Pleiades Publishing, Ltd., 2008.
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BASIC RESEARCH

A Study of the Transport of Charge Carriers in Coupled Quantum Regions

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Submitted January 28, 2008

Abstract—Specific features of controlled relocation of charge carriers in nanostructures based on tunneling-coupled quantum regions formed by GaAs/AlGaAs heterojunctions are considered. The results of numerical simulation of dynamics of controlled tunneling relocation of the maximum in the amplitudes of wave functions of charge carriers are discussed.

PACS numbers: 73.21.Fg

DOI: 10.1134/S1063782608130022

One of the promising lines in the development of nanodimensional components consists in the formation of structures based on tunneling-coupled quantum regions formed by GaAs/AlGaAs heterojunctions. In the context of this line, a number of semiconductor devices with high-speed response unlimited by the electrons' time of transit through active regions have been developed [1–3]. Operation of this class of devices is based on the principle of controlled relocation of the maximum in wave functions of electrons between tunneling-coupled quantum regions.

The aim of this study was to perform simulation of tunneling transport of charge carriers in coupled quantum regions formed by GaAs/AlGaAs heterojunctions.

It was shown previously [3, 4] (when considering nanostructures based on tunneling-coupled quantum regions) that controlled relocation of electrons in such quantum systems is complex and is governed not only by parameters of the tunneling barrier but also (to a considerable degree) by the energy spectrum of charge carriers and by the shape of pulses of the control voltage. In the case of steplike variation in the control voltage, the nondissipative relocation of electrons does not occur; rather, the system transfers to an excited state that is characterized by small-amplitude periodic oscillations of probability of finding the electrons in coupled quantum regions. In this case, the relocation process should be simulated with the energy relaxation taken into account.

According to [3, 4], the control pulse of the following complex shape should be applied in order to accomplish nondissipative relocation:

(i) at the initial point in time, the control voltage corresponding to equiprobable location of electrons in tunneling-coupled quantum wells is applied (in this case, periodic relocation of charge carriers between quantum regions); and

(ii) at the instant of time corresponding to the highest probability of finding an electron in the first quantum region and, consequently, to the lowest probability of finding the electron in the second quantum region, the control voltage should be increased steplike to the value that corresponds to relocation under the steady-state conditions, which hinders the reverse relocation.

In actual circuits, formation of such complex pulses is highly complicated and can represent a serious obstacle to realization of nanostructures with controlled relocation of maximum in the amplitude of the electron wave functions.

Konoplev and Ryndin [5] discussed a number of problems in realization of components that provide controlled relocation and are related to the use of only the channels with *n*-type conductivity: unacceptably low interference immunity; small logical difference; flow of through current under steady-state conditions; and a large ratio between the total number of electrons in coupled quantum regions in inverse stationary states, which limits the minimum time of delay of the component by the time of transit of charge carriers through active regions.

In order to solve the above problems, methods for fabricating nanodimensional components based on tunneling-coupled quantum regions with complementary conductivity types were suggested [5]. A combination of the principles of controlled tunneling relocation with complementary logic and also the paraphase control provide the retention of an invariant total number of mobile charge carriers in coupled quantum regions in the case of variation in the control voltages and make it possible to reduce the minimum delay time of devices

to values determined by the time required for tunneling relocation and provide an increase in the interference immunity, an increase in logical difference, and a decrease in the switching energy.

In Fig. 1, we show the structure and schematic diagram of an inverter based on tunneling-coupled quantum regions with the *n*- and *p*-type of conductivity [5]. Designations of external contacts in Figs. 1a and 1b (U_{dd} is the supply voltage, G_{nd} is the zero-potential bus, U_{in} is the input voltage, and U_{out} is the output voltage) correspond to the equivalent circuit shown in Fig. 1c, where the tunneling-coupled quantum regions are conditionally represented in the form of pairs of transistors that have corresponding conductivity type and are connected by dashed lines.

According to Figs. 1a and 1b, a tunneling-coupled nanostructure with a certain conductivity type is represented by two quantum wells that are identical in width and depth and are separated by a tunneling-transparent heterojunction barrier. The quantum wells have separate ohmic contacts for detection of the state of the quantum system and paraphase control of relocation of the largest amplitude of wave functions using both the Schottky gate at the upper face of the crystal and the control *p–n* junction on the side of the semi-insulating substrate. Ohmic contacts to the regions of the control *p–n* junctions are formed at the periphery of tunneling-coupled nanostructures and are not shown in Fig. 1. The heavily doped regions of ohmic contacts are separated by layers of wide-gap undoped GaAs with thickness approximately 20 nm in order to prevent the tunneling of charge carriers between these regions. The doped barrier regions *n*/*p*-$Al_{0.3}Ga_{0.7}As$ are separated from the *i*-$Al_{0.3}Ga_{0.7}As$ quantum wells by spacers in order to reduce the scattering of mobile charge carriers in the case of longitudinal transport in quantum wells by long-range Coulomb potential of impurity ions.

Konoplev and Ryndin [5] reported the results of numerical simulation of components based on tunneling-coupled quantum regions with complementary conductivity types; according to these results, as the control voltages are changed by the value of logical difference, an irreversible nondissipative tunneling relocation of the maximum of amplitudes of the wave functions of charge carriers in coupled quantum regions occurs with a delay shorter than 0.2 ps. Comparison of these results with those obtained by Gorbatsevich et al. [3, 4] requires conduction of additional simulations in order to reveal specific features of tunneling-coupled nanostructures that make possible the nondissipative relocation of charge carriers and also the causes of irreversibility of the controlled relocation of the maximum of the amplitude of wave functions of charge carriers under the condition that such nondissipative relocation is feasible.

An analysis of specific features of controlled relocation of the maximum in the amplitude of wave functions in tunneling-coupled quantum regions was performed for nanostructures shown in Fig. 1a, under the assumption of steplike variation in the paraphase control voltages according to the results of numerical solution of the time-dependent Schrödinger equation [4]:

$$-i\hbar\frac{\partial\Psi}{\partial t} = \frac{\hbar^2}{2}\frac{\partial}{\partial x}\left(\frac{1}{m^*(x)}\frac{\partial\Psi}{\partial x}\right) - V\Psi)(x, t),$$

where x is coordinate; t is time; $\Psi(x, t)$ is the wave function of an electron; V is the potential energy; m^* is the effective mass of the charge carrier; i is the imaginary unit; and $\hbar$ is Planck's constant.

The energy spectrum and wave functions at the initial point in time were determined from the self-consis-

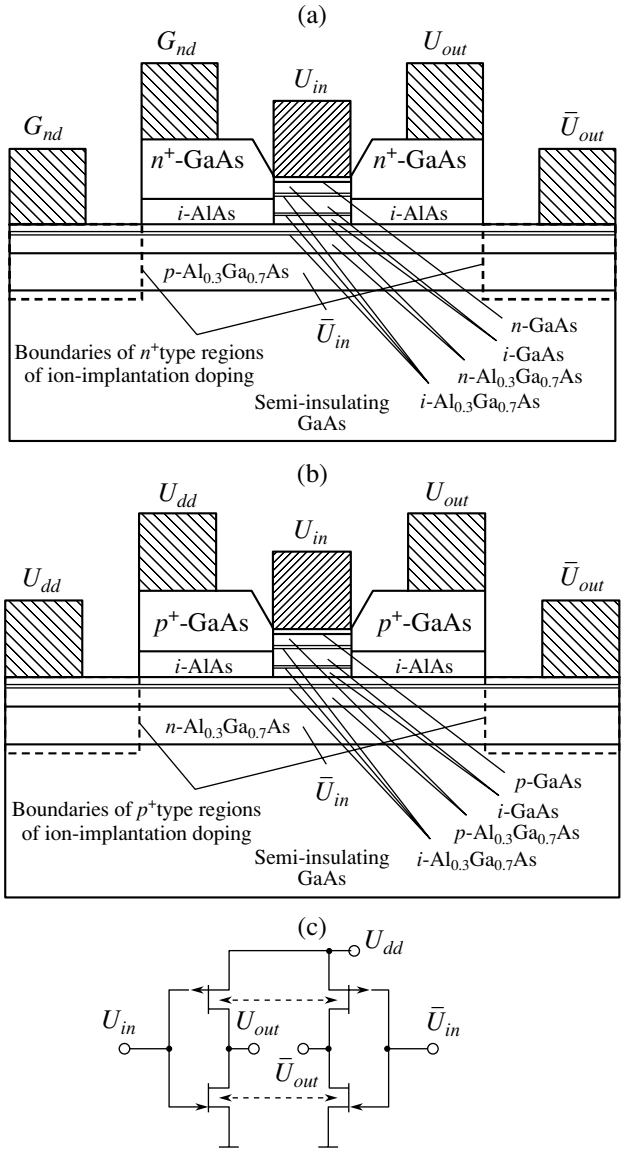

Fig. 1. The structure of an inverter based on tunneling-coupled quantum regions with (a) *n*-type and (b) *p*-type conductivity and (c) equivalent circuit of the inverter [5].

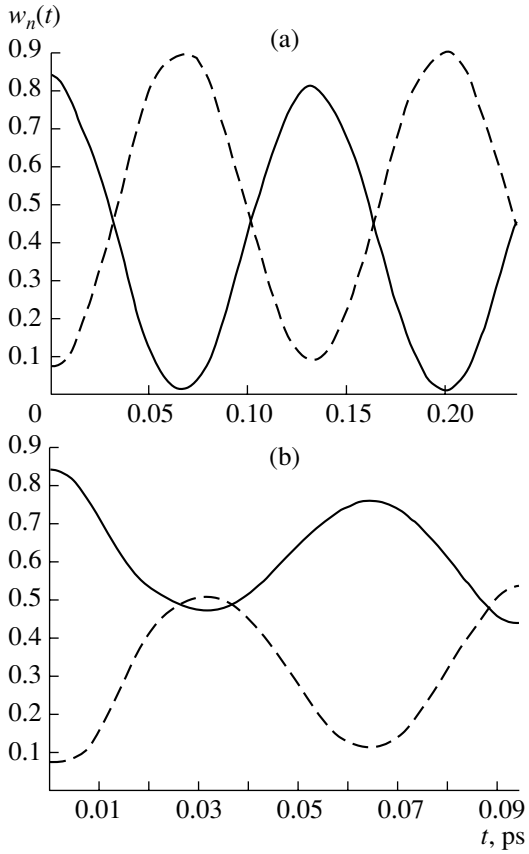

Fig. 2. Time dependences of probabilities of finding electrons in the 5-nm-wide tunneling-coupled quantum regions in the case of steplike variation in the control voltage U (*a*) from 0.5 V to 0 V and (*b*) from 0.5 V to –0.5 V (the solid line corresponds to —— $w_{n1}(t)$, while dashed line corresponds to–– $w_{n2}(t)$).

tent solution of the Poisson equation and time-independent Schrödinger equation according to [2, 6]. At the boundaries of the simulation region (boundaries of controlling junctions), the Dirichlet conditions were specified as

$$\Psi(x_{\min}, t) = \Psi(x_{\max}, t) = 0,$$

where $x_{\min}$ and $x_{\max}$ are coordinates of boundaries of the simulation region.

In Fig. 2, we show the temporal dependences of probabilities of finding electrons in tunneling-coupled quantum regions of a nanostructure based on $GaAs/Al_{0.3}Ga_{0.7}As$ heterojunctions with the width of quantum wells 5 nm, width of tunneling barrier 2 nm, and width of barrier regions of control junctions 30 nm in the case of steplike (during one step of increment in time) variation in the potential difference between control gates $U = U_{in} - \overline{U}_{in}$ (see Fig. 1) from 0.5 to 0 V and from 0.5 to –0.5 V.

These results were obtained using an inhomogeneous coordinate grid that contained 30 steps per each structural layer of semiconductor; the step of increment in time 0.01 fs. The minimum step of energy in solving the time-independent Schrödinger equation was 7×10^{-9} eV.

The initial control potential difference $U = 0.5$ V corresponds to the maximum probability of finding electrons in the upper (in Fig. 1a) quantum well and, consequently, corresponds to the minimum probability of finding charge carriers in the lower quantum well. Taking into account the symmetry of the nanostructure under consideration (equal values of the parameters of quantum regions above and below the tunneling barrier in the cross section), we realize that the control voltage $U = 0$ corresponds to an equal probability of finding electrons in the upper and lower quantum wells. In this case, if the energy relaxation is not taken into account, one observes (as should be expected) a periodic relocation of the maximum of amplitudes of carrier wave functions, which, according to Fig. 2a, manifests itself in large-amplitude oscillations (with a period of 130 fs) in probabilities of finding electrons in tunneling-coupled quantum regions.

Since the model representation under consideration does not take into account the energy relaxation, as the potential difference between control gates is varied from 0.5 to –0.5 V (i.e., as the direction of the control field is changed without varying its absolute value), one should expect either an absence of relocation of the maximum of the amplitude of wave functions with a transition of the system to an excited state or (at certain arrangement of energy levels) a periodic relocation (as in the previous case) but with a shorter period, taking into account the presence of an electric field and the finite character of the wave-packet motion. The plots shown in Fig. 2a confirm that the system transfers to an excited state; oscillations of probabilities of finding electrons in connected quantum regions with a period of approximately 65 fs are observed. The amplitude of these oscillations is small and the maximum of the wave function remains for the main fraction of time in the upper quantum region; i.e., a nondissipative relocation does not occur.

Taking into account that it is practically impossible to accomplish a steplike variation in the control voltage for the above time (0.01 fs), it is expedient to consider the specific features of controlled relocation in the case of linear variation in the voltage with more realistic duration of the fronts. According to the results reported in [3, 4], it is possible to attain a nondissipative relocation in a time shorter than 1 ps in the case of linear application of the control voltage.

In Fig. 3, we show the temporal dependences of probabilities of finding electrons in the tunneling-coupled nanostructure in the case of linear variation in the control potential difference U from 0.5 to –0.5 V with various durations of the fronts.

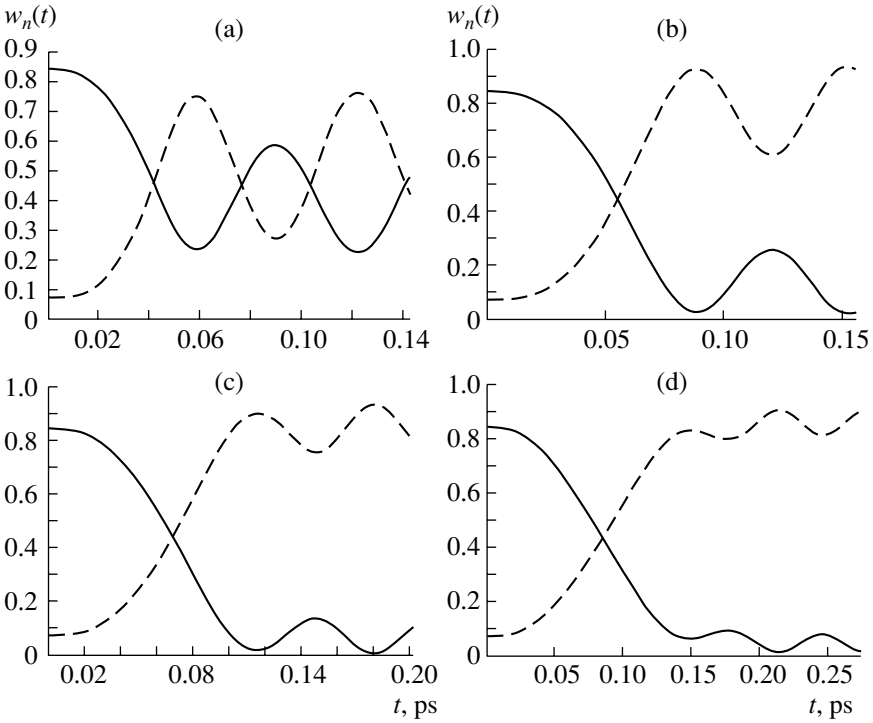

Fig. 3. Time dependences of probabilities of finding electrons in the 5-nm-wide tunneling-coupled quantum regions in the case of linear variation of U from 0.5 to –0.5 V and the front duration (a) 50, (b) 100, (c) 150, and (d) 200 fs (the solid line represents —— $w_{n1}(t)$, while the dashed line represents—- $w_{n2}(t)$).

According to Fig. 3a, at the front duration of 50 fs, the amplitude of oscillations of probabilities increases owing to an increase in the time of residence of the quantum system in the vicinity of the state corresponding to the resonance of states; this effect corresponds to partial periodic relocation of the maximum of the amplitude of wave functions between coupled quantum regions.

If the front durations are 100 fs or longer (Figs. 3b, 3c, 3d), the duration of finding the quantum system in the vicinity of the state corresponding to a resonance of the levels increases even more. In addition, at the instant of completion of the control pulse, an almost complete relocation of the maximum of the amplitude of the wave function occurs. As a result, after completion of the pulse's leading edge, reverse relocation is not observed (in contrast to Fig. 3a) even without consideration of dissipative processes. Rather, only oscillations in the probabilities of finding the charge carriers in coupled quantum regions are observed; the amplitude of these oscillations decreases as the duration of the control-pulse front is increased.

The time of irreversible relocation of the maximum of wave functions as the duration of control-pulse fronts is increased from 100 to 200 fs also increases from 75 to 130 fs (at the probability levels 0.1 and 0.9), respectively (Figs. 3b, 3c, 3d).

It is also worth noting that, in this case, irreversible character of nondissipative relocation is promoted by the symmetry of the nanostructures under consideration (equal values of parameters of the quantum regions) and paraphase control, which give rise to identical values of the system's energy in opposite stationary states and are conducive to a decrease in the energy of switching.

An increase in the width of quantum regions leads to a drastic decrease in the intensity of scattering of charge carriers at heteroboundaries and makes it possible to increase significantly the mobility of charge carriers in the case of longitudinal transport in quantum wells [7]. As a result, it is of interest to consider specific features of controlled relocation in wider coupled quantum regions.

In Fig. 4, we show the time dependences (similar to those considered above) of probabilities of finding electrons in tunneling-coupled quantum wells with 10-nm width in the case of linear variation in the control potential difference from 0.5 to –0.5 V with various durations of the fronts.

In this situation, in contrast to narrow quantum wells, relocation of the maximum of the wave-function amplitude is observed even in the case of practically steplike variation in the controlling voltage (Fig. 4a). The relocation time is approximately 110 fs and the oscillation period is 220 fs. These results are accounted for by an increase in the number of allowed energy lev-

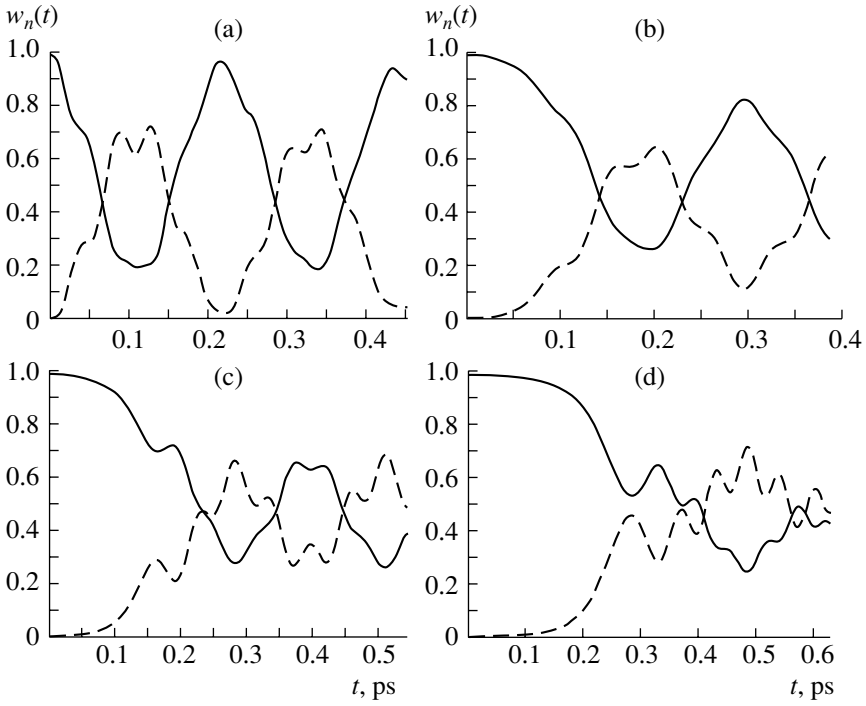

Fig. 4. Time dependences of probabilities of finding electrons in the 10-nm-wide tunneling-coupled quantum-regions in the case of linear variation in U from 0.5 to –0.5 V and the front durations (a) 0.1, (b) 100, (c) 200, and (d) 400 fs. The solid line represents —— $w_{n1}(t)$, while the dashed line represents—- $w_{n2}(t)$.

els in quantum regions and, consequently, by an increase in the number of resonances for these levels as the control voltage is varied. An increase in the oscillation period compared to Fig. 3 corresponds to the increase in the quantum-well width from 5 to 10 nm with invariable parameters of the tunneling barrier and barrier regions of controlling junctions.

As the duration of fronts of the control pulses is increased, the amplitude of oscillations in the maximum of the wave functions decreases relative to the equilibrium positions, as in the case of narrow quantum wells (see Fig. 4). However, as a result of the increase in the number of allowed levels in quantum regions in this case, oscillation of probabilities of finding the charge carriers are observed in the vicinity of the value of 0.5, which gives rise to reversible partial relocation. In addition, further small-amplitude oscillations with a period of about 60 fs are observed.

In Fig. 5, we show separate generalized characteristics of the process of controlled tunneling relocation of the maximum of wave functions of charge carriers in relation to parameters of the nanostructure and control signal; these characteristics were obtained for tunneling-coupled quantum regions that had a width of 10 nm and were separated by a 2-nm-thick tunneling barrier.

Dependences of averaged probabilities for finding electrons in tunneling-coupled quantum regions $\langle w_1 \rangle$ and $\langle w_2 \rangle$ and the amplitudes of oscillations A_P on the amplitude of control pulses U and the width of the barrier regions in control junctions W_B shown in Figs. 5a, 5b, and 5d are obtained at a duration of the controlling-pulse front 100 fs and reflects the pattern observed after completion of the given control front.

An analysis of the above results of numerical simulation makes it possible to advance the following conclusions:

(i) In fairly narrow (with the width of about 5 nm) tunneling-coupled quantum regions, a steplike variation in the control voltage does not result in relocation of the maximum of the wave function amplitude for the charge carriers. The system is transferred to an excited state while relocation occurs owing to dissipative processes.

(ii) In the case of linear variation in the control potential difference, due to

an increase in the time of finding the quantum system in the vicinity of the state that corresponds to resonance of the levels, the nondissipative relocation of the maximum of wave-function amplitudes occurs between coupled quantum regions; this relocation is irreversible even with dissipative processes disregarded if the duration of the control-pulse fronts is no shorter than 100 fs. In this case, oscillations of probability of finding the charge carriers in coupled quantum regions are observed; the amplitude of these oscillations decreases as the duration of fronts of the control pulses is increased, in accordance with the dependence shown in Fig. 5c.

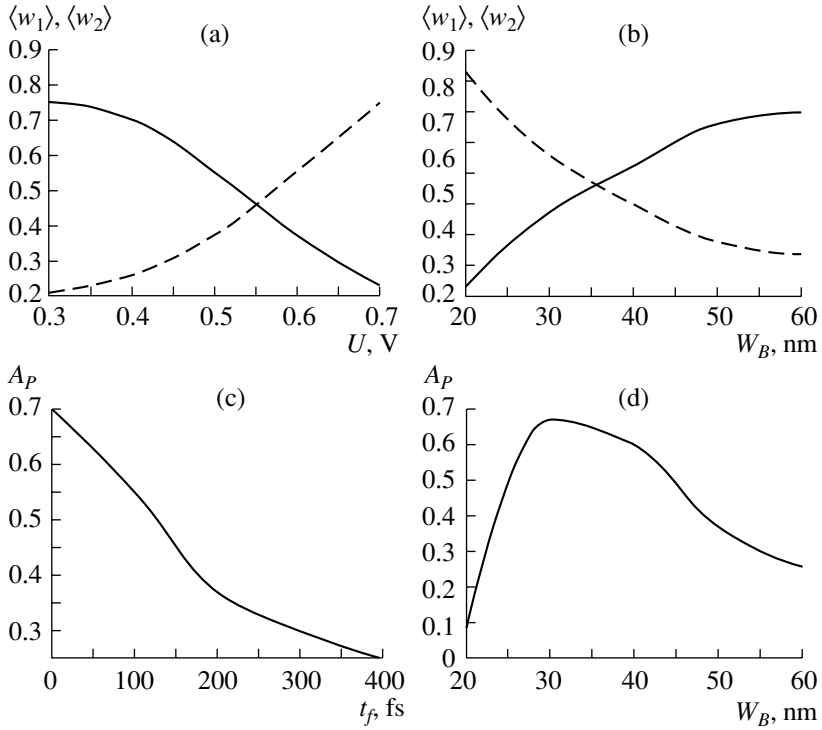

Fig. 5. Dependences of averaged probabilities of finding charge carriers in quantum regions on (a) the amplitude of a control pulse, (b) the width of barrier regions in controlling junctions, (c) amplitude of oscillations of probabilities of finding electrons in coupled quantum regions on (c) duration of the fronts of the control signal and (d) the width of barrier regions in control junctions.

(iii) Irreversibility of nondissipative relocation is favored by symmetry of nanostructures (equal values of parameters of the quantum regions) and the paraphase control, which provide equal values of energy of the system in opposite stationary states and favor a decrease in the power consumption.

(iv) As the width of tunneling-coupled quantum regions is increased (to 10 nm or larger), relocation of the amplitude maximum of wave functions is observed even in the case of steplike variation in the control voltage, which is accounted for by an increase in the number of allowed energy levels in the quantum regions and, consequently, an increase in the number of resonances of these levels in the course of switching.

(v) As the duration of the fronts of control pulses in coupled quantum regions with width no smaller than 10 nm increases, relocation of the maximum of the amplitude of wave functions is reversible due to an increase in the number of allowed levels.

(vi) Nondissipative relocation in a system of tunneling-coupled quantum regions is observed only if the amplitude of control pulses exceeds some value that depends on the nanostructure parameters. For example, if the width of quantum wells is 10 nm, the width of the tunneling barrier is 2 nm, and the width of the barrier regions in control junctions equals 30 nm, we use Fig. 5a to find that the difference between averaged probabilities of finding electrons in coupled quantum regions reverses its sign at an amplitude of control pulses in excess of 0.55 V. It is noteworthy that it is at this amplitude that the observed oscillations have the maximum swing and relocation is reversible.

(vii) The dynamics of the relocation process is governed to a great extent not only by the width of quantum wells and penetrability of the tunneling barrier but also by the width of barrier regions in control junctions as a result of the effect of reflection of wave functions of charge carriers from exterior boundaries (boundaries of control junctions). In accordance with the dependences shown in Fig. 5b, nondissipative relocation over averaged probabilities of finding the particles in coupled quantum wells is observed if the width of barrier regions in the control junctions is smaller than some value (for the nanostructure under consideration, smaller than 35 nm). In addition, as shown in Fig. 5d, it is at this width of barrier regions that the observed oscillations of probabilities have the largest amplitude and the relocation is reversible.

(viii) Taking into account that, even if the duration of fronts of control pulses is increased, relocation in coupled quantum regions with a width in excess of 10 nm is reversible, in this case, a more adequate consideration of dynamics of controlled relocation for actual devices is possible only if dissipative processes are taken into account.

This study was supported by the Ministry of Education and Science of the Russian Federation, grant no. 2007-3-1.3-11-03-005.

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Translated by A. Spitsyn

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