NUMERICAL SIMULATION OF THE RESONANCE-TUNNEL STRUCTURE BASED ON THE SCHOTTKY BARRIER AND A GaAs/AlGaAs HETEROJUNCTION

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The resonance tunneling diode has been widely studied because of its importance in the field of nanoelectronic technology and its potential applications in very high speed/functionality devices and circuits. Even though much progress has been made in this regard, the most popular structure of these diods consists of barriers created by heterojunctions only. In this paper, we present numerical simulation results for a two-barrier resonance-tunnel structure consisting of the Schottky barrier and a GaAs/AlGaAs heterojunction. We considered its potential application to the resonance-tunnel diodes working at room temperature. The configuration of this structure was optimized using numerical simulation methods. A current voltage characteristic was simulated by the example of the optimized structure, and the influence of the thermal current on the obtained dependence was analyzed.

Key words: numerical simulation; resonance-tunnel structure; Schottky barrier; heterojunction

Citation: A.S. Abrosimov, V.N. Agarev, Numerical simulation of the resonance-tunnel structure based on the Schottky barrier and a GaAs/AlGaAs heterojunction, St. Petersburg Polytechnical State University Journal. Physics and Mathematics. 11 (1) (2018) 5 – 12. DOI: 10.18721/JPM.11101

Introduction

Resonant tunneling diodes based on nanoscale semiconductor heterostructures have an *N*-shaped current-voltage characteristic (*I*–*V* curve) with a negative differential resistance region and short response times of the tunneling process (lasting on the order of 10^{-13} s). For this reason, these diodes show great potential for applications in high-speed terahertz devices and digital devices with switching times on the order of 10^{-12} s or less. Iogansen was the first to propose using the effect of resonant electron tunneling in layered thin-film metal–insulator structures for creating electronic interferometers, thin-film diodes, triodes, etc. [1 – 3].

Investigation of resonant tunneling structures

Ref. [4] studied the *I*–*V* curve of an $Al_{1-x}Ga_xAs/GaAs/Al_{1-x}Ga_xAs$ structure with different barrier thickness to quantum well ratios. Resonant current was observed only at low temperatures (77 K and below) for all structures under consideration; all effects associated with tunneling disappeared at room temperature. The authors explained this by thermal smearing of the local levels in the quantum well and by a low barrier which electrons whose energies are relatively high energies for room temperature pass through easily.

On the other hand, a decrease in temperature to 4.2 K does not lead to the expected ‘sharpened’ tunneling, which is probably due to scattering by structural fluctuations and impurities; this scattering also results in a broadening of the local levels.

A current peak caused by the resonant tunneling effect is observed on the *I*–*V* curve at 77 K, while the curve’s simulated shape agrees with the experimental one. This feature disappears at room temperature.

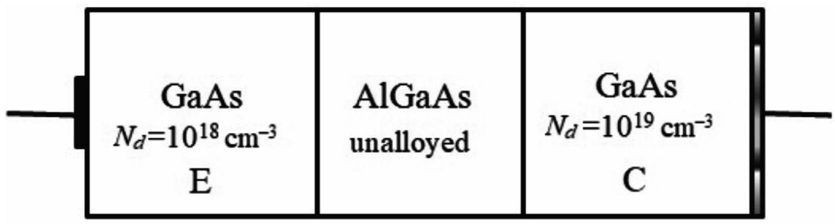

Fig. 1. Schematic of a resonant tunneling structure
GaAs collector metal (Schottky barrier); GaAs/AlGaAs heterojunction (the second barrier);
E and C are the emitter and the collector, respectively

Four factors influence the magnitude of the tunneling current [5]: the thickness of the barrier, the width of the well, the height of the barrier and the concentration of impurities in the contact region. While the first three factors determine the height of the peak and the behavior of the dependence of the transparency coefficient on the electron energy, the fourth one determines the energy distribution of these electrons at the input to the two-barrier structure.

The *I*–*V* curve of a resonant-tunnel diode is also affected by its material. For example, the height of the i_{max} peak for InAlAs/InGaAs structures is almost an order of magnitude higher than for AlAs/GaAs, with approximately the same i_{max}/i_{min} ratio [6]. Multi-barrier structures have also yielded good results. The electron energies in such a system containing a sequence of monotonically narrowing quantum wells are the same at equivalent levels of all wells [7]. This is achieved by tailoring the widths of the wells so that the value of the potential difference applied to the structure is equal to the height difference between the ground level of the narrowest quantum well and the Fermi level.

A sharp resonance peak is observed on the *I*–*V* curve of the structure at sufficiently low barrier permeability, when level splitting due to overlapping of electron wavefunctions in adjacent wells is small. This peak is formed by electrons whose energy lies in a narrow range near the ground state energy of the narrowest quantum well.

Simulation procedure

In this paper, we have investigated a two-barrier resonant tunneling structure where the Schottky barrier, which is natural for metal–gallium arsenide (GaAs) contact and caused by surface states, is necessarily present (Fig. 1). Its height for various metals is about 0.8 eV [8].

The second barrier is a GaAs/AlGaAs heterojunction, which can have different heights (depending on the aluminum fraction). The thickness of the AlGaAs layer responsible for the heterojunction barrier width is also varied.

We assumed that the carrier density n reached 10^{19} cm^{-3} for the simulated structure. The Schottky barrier with such an impurity concentration has the smallest thickness, and this concentration is technologically obtained with the least number of implantation defects.

Within our model, the region of the Schottky barrier is a depleted layer, so the distribution of external potential is assumed to be linear, with its maximum at the point $x = 0$, and its zero at the metal–semiconductor interface (Fig. 2). The external voltage falls between the Schottky barrier (this is a metal–GaAs transition, which is a collector) and the heavily doped GaAs region which serves as the second contact. The structure’s emitter is located on the left, on the side of the heterojunction barrier, and the collector is on the right, the side of the Schottky barrier (see Fig. 1).

In practice, it is possible to create resonant tunneling diodes with heterojunction barrier heights up to 0.4 eV. This limit is due to recombination centers emerging in a semiconductor, and, as a consequence, high noise on the *I*–*V* curve of the structure.

In this study we have analyzed resonant tunneling structures with barrier heights from 0.3 to 0.4 eV. The current in these structures was calculated as created by electrons moving from the emitter to the collector [5]; as a result, its density followed the expression

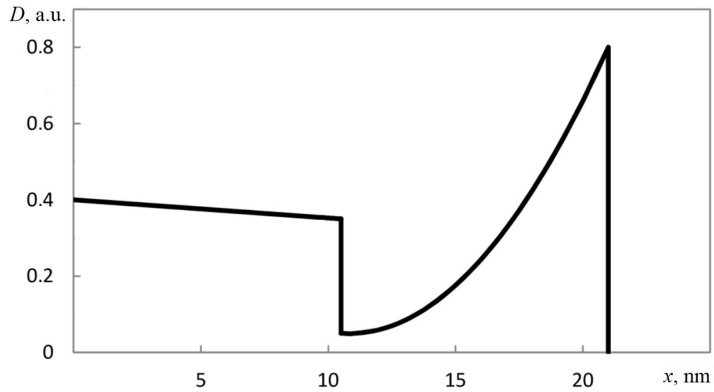

Fig. 2. The energy diagram of the structure with an external voltage of 0.1 V applied

$$j = \frac{em^* k_B T}{2\pi^2 \hbar^3} \int_0^\infty D(E) \times \\ \times \ln\left[1 + \exp\left(\frac{E_F - E}{k_B T}\right)\right] dE - \\ - \frac{em^* k_B T}{2\pi^2 \hbar^3} \int_0^\infty D(E) \times \\ \times \ln\left[1 + \exp\left(\frac{E_F - E - eV}{k_B T}\right)\right] dE, \quad (1)$$

where E is the energy; V is the voltage applied to the structure; $D(E)$ is the transmission coefficient; E_F is the energy of the Fermi level; T is the temperature;

k_B is the Boltzmann constant; e and m^* the electron charge and effective mass.

The E_F value is determined from the solution of the electroneutrality equation

$$\frac{N_d}{1 + \beta^{-1} \exp\left(\frac{E_F - E_d}{k_B T}\right)} = N_c F_{1/2}\left(\frac{E_F}{k_B T}\right), \quad (2)$$

where β is the spin degeneracy factor ($\beta = 1/2$); N_d is the donor impurity concentration ($N_d = 10^{19}$ cm^{-3} in the present study, it is taken for the GaAs layer adjacent to the Schottky barrier); N_c is the effective density of states in the conduction band; $F_{1/2}$ is the Fermi integral with the index 1/2; E_d is the energy of the donor level.

The donor level in gallium arsenide is created by silicon with a depth of −6 meV relative to the bottom of the conduction band. We obtained the $D(E)$ dependence by the method proposed in [9], by solving the Schrцdinger equation in the one-electron approximation without scattering effects taken into account.

Let the two-barrier structure be located at distances from 0 to L; then the wave function is taken from the Schrцdinger equation:

$$\psi'' + \frac{2m^*}{\hbar^2}(E - U(x))\psi = 0, \quad (3)$$

where m^* is the effective electron mass (for simplicity, it is assumed to be the same in the entire region under consideration).

The solution of the equation in the outer regions are functions of the following form:

$$x \le 0, \quad \psi = e^{ikx} + re^{-ikx}; \\ x \ge L, \quad \psi = de^{ik(x-L)}, \quad (4)$$

where r and d are the amplitudes of reflection and transmission, respectively; k is the wave vector magnitude.

The reflection and transmission coefficients follow the expression

$$R = |r|^2, D = |d|^2, \quad (5)$$

The boundary conditions are obtained from functions (4):

$$\psi(0) = 1 + r, \quad \psi(L) = d, \\ \psi'(0) = ik(1 - r), \ \psi'(L) = ikd. \quad (6)$$

Let us express the amplitudes r and d through functions $\psi(0)$ and $\psi(L)$; the boundary conditions can be then written as

$$\psi'(0) + ik\psi(0) = 2ik, \\ \psi'(L) - ik\psi(L) = 0. \quad (7)$$

Equation (3) together with conditions (7) determine the problem in the inner region at distances from 0 to L. Solving this problem and finding $\psi(x)$, we can find the reflection and transmission coefficients in the following form:

$$D = |d|^2 = |\psi(L)|^2,\ R = |r|^2 = |\psi(0) - 1|^2. \quad (8)$$

Let us take the structure's total length L for unity, then the Schrцdinger equation takes the form

$$\psi'' + (\varepsilon - U(x))\psi = 0, \quad (9)$$

where the energy ε and the potential $U(x)$ are counted in units $\hbar^2 / 2mL^2$.

Let us divide the section from 0 to L into N regions of length a. Then $L = Na$; if $L = 1$, then $a = 1/N$.

For an arbitrary point inside the region, equation (9) can be written in a discrete form:

$$\psi_{n+1} + \psi_{n-1} + \varepsilon_n\psi_n = 0, \quad (10)$$

$$\varepsilon_n = -2 + a^2(\varepsilon - V_n). \quad (11)$$

For the first of boundary conditions (7), let us replace the wave function derivative with its discrete equivalent

$$\psi'(0) \approx (\psi_1 - \psi_{-1}) / 2a.$$

Then the boundary condition and the Schrцdinger equation for $x = 0$ have the form

$$\begin{aligned} \psi_1 - \psi_{-1} + 2ika\psi_0 &= 4ika, \\ \psi_1 - \psi_{-1} + \varepsilon_0\psi_0 &= 0. \end{aligned} \quad (12)$$

Adding up the two equations of (12) and dividing this sum by 2, we obtain the first boundary condition:

$$\psi_1 + \left(\frac{\varepsilon_0}{2} + ika\right)\psi_0 = 2ika. \quad (13)$$

For the second boundary condition ($x = N$), we similarly find:

$$\begin{aligned} \psi_{N+1} - \psi_{N-1} - 2ika\psi_N &= 0, \\ \psi_{N+1} - \psi_{N-1} + \varepsilon_N\psi_N &= 0, \end{aligned} \quad (14)$$

and from this we obtain this condition in the form

$$\psi_{N-1} + \left(\frac{\varepsilon_N}{2} + ika\right)\psi_N = 0. \quad (15)$$

Thus, the problem consists in solving the system of equations (10), (13), and (15).

The tridiagonal system of equations (10) is solved by the modified sweep method [10].

Results and discussion

At the first stage of the simulation, the resonant tunneling structure was optimized based on the transmission coefficient $D(E)$ depending on the width and height of the GaAs/AlGaAs heterojunction barrier; we selected the geometric parameters (height and width) of this barrier with which the transmission coefficient took the greatest value, at least 70 %.

An example of the simulation result is shown in Fig. 3. Notice that the barriers in this structure are rather wide (up to 11 nm) and the width of the peaks on the $D(E)$ dependence does not exceed several tens of millielectronvolts (specifically, it was varied from 0.01 to 20 meV). The $D(E)$ dependences we have obtained did not take into account the scattering effects in solving the Schrцdinger equation in the one-electron approximation with the help of the above-described numerical method.

The highest transmission coefficients were observed in structures with Schottky barrier heights of 0.30 – 0.35 eV and widths of 6 – 9 nm. The transmission coefficient was more than 95 % in some of these structures. Additionally, resonant tunneling with peaks of 10 % or higher was observed for all configurations of the heterojunction barrier.

Fig. 4 shows examples of the dependence of the maximum value of the transmission coefficient on the external voltage with varying barrier width (from 6 to 11 nm) and fixed barrier height (0.4 eV). As the width of the barrier decreased, the height of the peaks increased; the form of the dependence changed from decreasing at the maximum width to increasing (up to the value of the transmission coefficient over 90 %).

An examination of the selected models of resonant tunneling structures revealed that the transmission coefficient value depends more on the height of the heterojunction barrier than on its width. The transmission coefficient values determine the simulated behavior of the I–V curve of the resonant tunneling diode (see Eq. (1)); however, while analysis of these coefficients is important, it does provide a

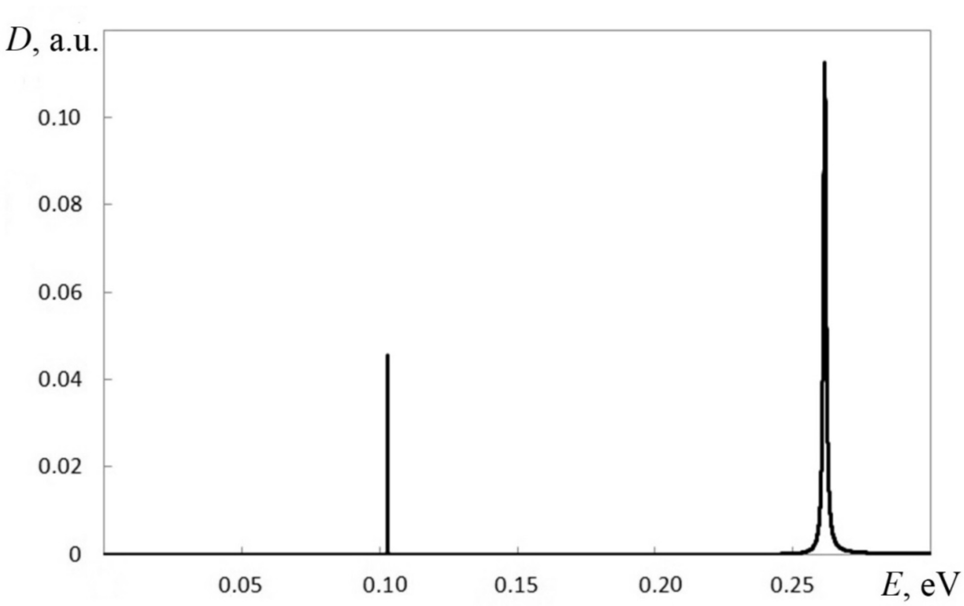

Fig. 3. Transmission coefficient versus energy with a heterojunction barrier width of 6 nm and height of 0.3 eV (the result of simulation)

complete picture of the optimization. For this reason, we also simulated the *I*–*V* curves of these structures at two temperatures: 100 and 300 K.

Fig. 5 shows the *I*–*V* curves of a resonant tunneling structure with a barrier height of 0.3 eV and a thickness of 6 nm; the highest and broadest current peak is observed at these parameters. The calculated *I*–*V* curves were obtained at 100 and 300 K.

It can be seen from the dependences that the current density peak reaches a value that is acceptable for experimental observation (up to 10^8 A/m^2) at 300 K. The current density for the resonant tunneling structures under

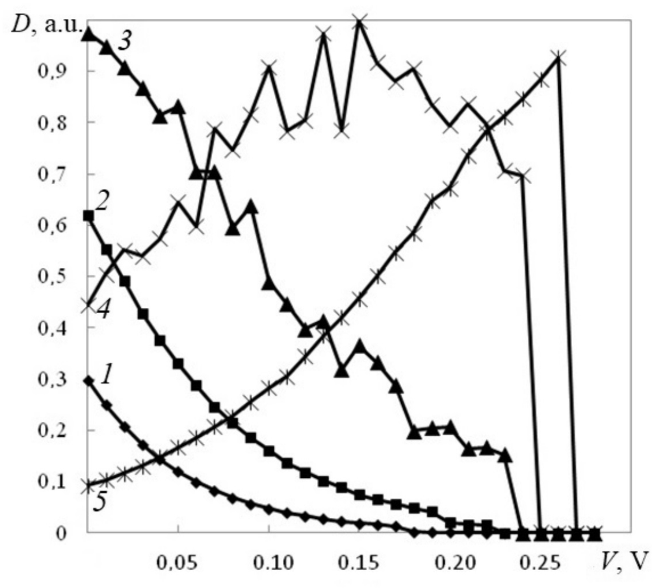

Fig. 4. Dependences of the maximum transmission coefficient on the external voltage with a variation in the heterojunction barrier width, nm: 11 (curve *1*), 10 (*2*), 9 (*3*), 7 (*4*), 6 (*5*); barrier width was 0.4 eV

consideration has two components at nonzero temperatures, the thermal and the tunneling one. The tunneling current has been discussed above, and the thermal current is expressed by the following formula:

$$j_{therm} = ne\left(\frac{k_B T}{2\pi m^*}\right)^{1/2} \exp\left(-\frac{e\varphi}{k_B T}\right)\times \left(\exp\left(\frac{eV}{k_B T}\right)-1\right). \quad (16)$$

As a result, the current density J is expressed by the sum

$$J = j_{therm} + j_{tunnel} \quad (17)$$

where j_{tunnel} is the tunneling current density (1).

Due to the high Schottky barrier (φ = 0.8 eV), the thermal current injected through it is extremely small compared to the tunneling current. The thermal component at room temperature (300 K) is two orders of magnitude lower than the tunneling one.

The *I*–*V* curves shown in Fig. 5 were obtained without taking into account the effects of electron scattering. The main contribution to the current is made by resonant tunneling through the second level (see Fig. 3), for which the transmission coefficient peak is much wider and higher.

However, electron scattering in doped gallium arsenide can significantly affect the values of the transmission coefficient and current. This effect can be estimated by assuming that the transmission coefficient peak is described by the Lorentz formula [11]:

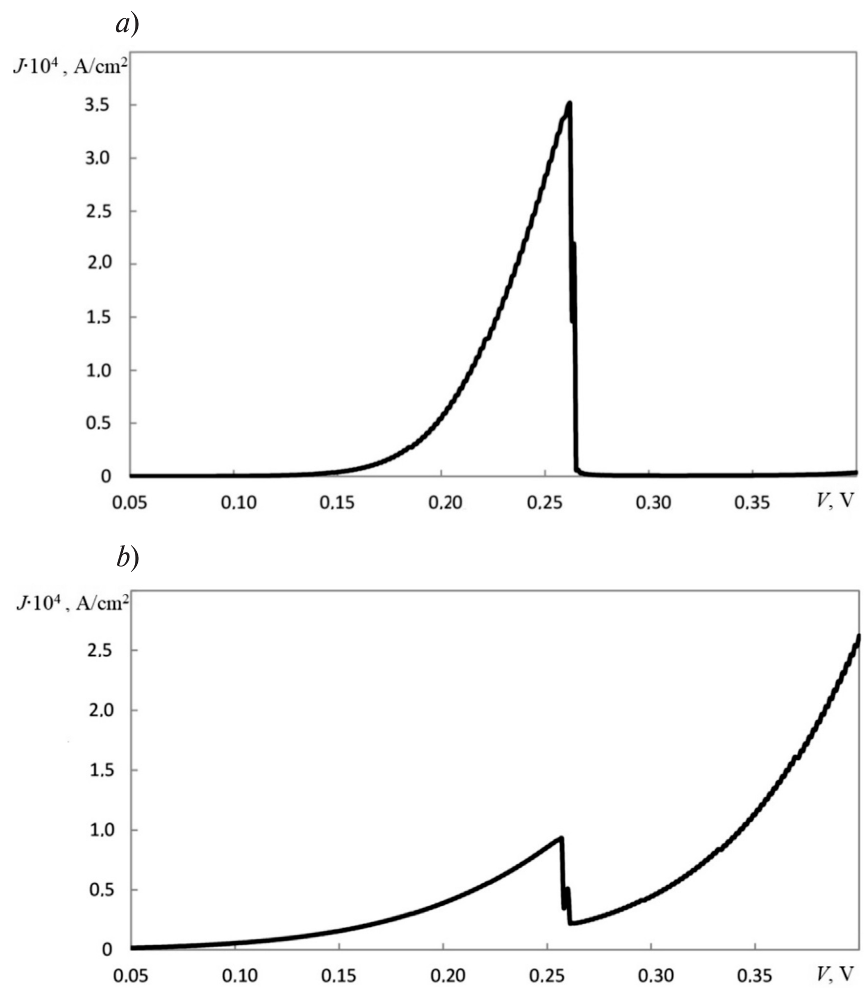

Fig. 5. *I*–*V* curve of a resonant tunneling structure with the heterojunction barrier width of 6 nm and the height of 0.3 eV at temperatures of 100 K (*a*) and 300 K (*b*)

$$D(E)=\frac{4D_1D_2}{(D_1+D_2)^2}\frac{\Delta E_b^2}{\Delta E_t^2+4(E-E_p)^2}, \quad (18)$$

where D_1 and D_2 are the coefficients of transmission through the first and the second barrier; ΔE_t is the total width of the peak; ΔE_b is the peak width without taking into account the scattering processes, E_p is the position of the maximum peak value.

The full width of the peak

$$\Delta E_t = \Delta E_b + \Delta E_r,$$

where ΔE_r is the width of the peak caused by relaxation processes; $\Delta E_r = \hbar / \tau_r$ (τ_r is the momentum relaxation time).

If we assume that electron mobility in doped gallium arsenide is $\mu = 0.4$ m^2/(V·s) at 300 K, then $\tau_r = 1.5 \cdot 10^{-13}$, $\Delta E_r = 4.4$ meV.

Thus, the influence of scattering processes manifests in a decrease in the height of the transmission coefficient peak by 4.4 times and in its broadening by 2.1 times. This should lead to a significant decrease in the tunneling current (current should decrease due to a decrease in the height of the resonant peak, but this decrease should be partially compensated by its broadening).

To estimate the effect of scattering on negative differential conductivity (NDC), we can assume that its maximum value $g_{\max}$ is proportional to the ratio $\Delta E_b^2 / \Delta E_t^2$, and then $g_{\max}$ will decrease by 4.4 times.

The above estimates prove that the effect of scattering in the structure under consideration reduces the peak current on the *I*–*V* curve by several times and expands the NDC region, making the current decay slower compared with the *I*–*V* curve in Fig. 5

However, NDC at normal temperature and the simplified technology (compared with a two-barrier heterostructure) are still important for practical applications, in comparison with a two-barrier heterostructure.

Conclusion

The paper presents the results of numerical simulation of promising resonant tunneling structures. We have established that tunneling effects in these structures persist at high temperatures up to room temperature, while the position and shape of the current density peak change with the configuration, i. e., the height and width of the GaAs/AlGaAs barrier of the resonant tunneling structure.

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Received 18.06.2016, accepted 24.10.2017.

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