Tunnelling transport in nonuniform barriers as a possible way for current control

V.A. Kozlov and V.A. Verbus
Institute for Physics of Microstructures, Russian Academy of Science, 603950 Nizhny Novgorod, GSP-105, Russia
kozlov@ipm.sci-nnov.ru

Abstract. This paper presents the results of computer simulation of the under barrier tunnelling transport through the nonuniform heterostructure barriers containing spherical or cylindrical nano objects. Embedding of nano objects in the barrier enables one to construct the semiconductor barriers with predefined properties. Application of external potential to these objects exponentially changes the current through the barrier and it can be used for current control and amplification of signals.

1. Introduction
The scale reduction of semiconductor devices requires the decrease of barrier dimensions. In the short part of nanometer range the semiconductor barriers produced by the bandgap engineering are nonuniform in plane. This can lead to new features of the hot electron transport in device. The aim of this paper is the simple quantum description of the tunneling transport [1] in the semiconductor barriers containing nano objects of spherical or cylindrical shapes. It is very useful for construction of new semiconductor devices with the external control of tunneling current.

In a conventional type FET, the electron transport in a channel along \( z \) direction is described by propagating Bloch waves \( a_k \exp(ikz) \), where \( k \) is the wave vector and \( a_k \) is the amplitude. To change the current we need to change the width of the channel by gate potential. This corresponds to the change in the number of propagating modes. It leads to linearly dependence of the current on a channel width. In contrast to this description, the tunneling current through the barrier is described by the exponential damping wave functions \( a_k \exp(-\eta z) + b_k \exp(+\eta z) \), where \( a_k \) and \( b_k \) are the amplitudes of forward and backward damping waves \( (k = i\eta) \). In this case a change in the barrier height leads to the correspondent change of the exponent power \( \eta z \) and the current control becomes more effective. So the question is: how to change the barrier potential by applying external voltage.

To realize this control we considered the semiconductor barrier with the built-in nanoscale objects. Two shapes of objects were considered: spherical and cylindrical. The potential of the spherical object which is embedded in a channel may be changed, for example, by the gate potential. The potential of cylindrical one may be changed by applying voltage to the end of the cylinder. The influence of spherical objects on the current was described by the application of the Mie theory [2] for the
scattering of electromagnetic waves by sphere. The cylindrical objects were described similarly. To calculate the current in the barrier we took into account both the forward and the backward waves.

2. Gamow Peak and Gamow Window

It is well known that tunneling processes in quantum mechanics were firstly introduced by George Gamow [3]. Now in nuclear and stellar physics the terms Gamow peak (Gp) and Gamow window (Gw) are frequently used for the description of penetration of the ensemble of carriers through the barrier. The term Gp denotes the carrier energy corresponding to maximum of tunneling penetration probability, and Gw is the energy interval corresponding to half maximum of this probability. The carriers in the ensemble are in thermal equilibrium with temperature T. The Gp arises due to the multiplication of two factors. The first factor is the tunneling transmission coefficient which increases with the increase of carrier energy. The second one is the Maxwell-Boltzmann or Fermi distribution function which decreases with the decrease of energy. It means that the Gp isn’t a resonance type and at adverse conditions it can be rather wide or absent. It is interesting to compare the conditions of existing Gp in stars and heterostructures. For example the temperature of the internal silicon shell of iron core in the supernova (type II) star is approximately equal to several T9 (where T9 = 10^9 K). If we estimate a typical nuclear potential V_nuc to be several MeV, and a typical bandoffset in heterostructures V_hs to be 100 meV, then we obtain the realistic temperature of heterostructure: T_hs = T9 (V_hs/V_nuc) = T2 = 100 K. This demonstrates common features in the different branches of hot carrier physics.

Consider the plane heterostructure barrier of thickness d with the flat barrier potential equal to \( V_b \). The wave function of carrier inside the barrier consists of the sum of two damping components. The first component exponentially increases in forward direction, but the second increases in the opposite direction. It corresponds to the distribution of minority carriers inside the base of bipolar transistor and one may hope to obtain the amplification of signal if it will be possible to change the barrier potential. Note that for calculation of the current it is necessary to take into account both forward and backward waves. To describe the tunneling transmission, it is useful to introduce the thickness potential \( V_d \) by the formula: \( V_d = \hbar^2 / (2 m^* d^2) \) so that \( V_d \) depends only on thickness d and effective mass \( m^* \). The tunneling transmission coefficient \( T_{\text{run}} \) for carrier with energy \( E \) through the barrier (for small transmission) can be written in the form:

\[
T_{\text{run}}(E) = 16 \frac{E}{V_b} \left( 1 - \frac{E}{V_b} \right) \exp \left( -2 \sqrt{\frac{V_b - E}{V_d}} \right).
\]

Thus the dependence of penetration probability for ensemble of carriers with temperature \( T \) versus energy is proportional to \( P(E) = T_{\text{run}}(E) \exp(-E/V_t) \), parameter \( V_t = k_B T \) is the so called thermal potential, \( k_B \) is the Boltzmann constant. The penetration probabilities for two heterostructure barriers with the same thickness (d = 10 nm) and effective mass (\( m^* = 0.1 m_n \)) for temperature (\( T = 100 K \)), are shown in figures 1 and 2. The only difference is the value of barrier potential: \( V_b = 100 \) meV for figure 1 and \( V_b = 200 \) meV for figure 2. These figures are very much alike and the main difference is in the penetration rates. The fall-off in penetration is equal to 160 times when the barrier potential increase is equal to 2 times. So it is possible to get the signal amplification. Especially, effective current control will be achieved if we build-in resonance levels into the barrier and the Gamow peak and resonance level coalesce together. The penetration of carriers through Gw produces the inverted distribution of transmitted carriers and a high frequency negative differential conductivity may arise.

3. Under barrier tunnelling transport with built-in spherical or cylindrical nano objects.

To describe the tunnelling transport through the barrier with embedded spherical (or cylindrical) object (considering as scatterer) we solved the Mie problem [2] in the single scattering approximation.
In our approach the scatterer contained the radial dependent potential which was approximated by the step function with constant potential inside each shell layer. The wave function \( \psi_j(r, \theta) \) inside the shell layer \( j \) was taken in the following form:

\[
\psi_j(r, \theta) = \sum_{l=0}^{\infty} (c^{(1)}_{jl}(\theta)h^{(1)}_l(k_j r) + c^{(2)}_{jl}(\theta)h^{(2)}_l(k_j r))
\]

(2)

where \( r \) is a radius from the centre of the scatter in a spherical coordinate system, \( \theta \) is the angle, \( l \) is the index of spherical harmonic, \( c^{(1)}_{jl}(\theta) \) and \( c^{(2)}_{jl}(\theta) \) are the coefficients containing Legendre polynomials \( P_l(\cos \theta) \). The functions \( h^{(1)}_l(k_j r) \) and \( h^{(2)}_l(k_j r) \) are the spherical Bessel functions of the third kind describing diverge and converge spherical waves. The scatterer consists of several spherical layers and \( j \) is the index of the layer, \( k_j = (2m_j(E - V_j))/h^2 \) is the wave vector in the \( j \) layer.

Outside the scatterer we added to the expression (2) the actuate plain waves: \( A \exp(i k \cos \theta) + B \exp(-i k \cos \theta) \). The coefficients \( A \) and \( B \) are the amplitudes of forward and backwards plain waves, propagating along direction \( z = r \cos \theta \). We fulfilled the Sommerfield boundary conditions at infinity together with the boundary conditions \( \psi_j(r_j) = \psi_{j+1}(r_j) \) and \( (\partial \psi_j(r_j)/\partial r)/m_j = (\partial \psi_{j+1}(r_j)/\partial r)/m_{j+1} \). This gave us the possibility to calculate the coefficients \( c^{(1)}_{jl}(\theta) \) and \( c^{(2)}_{jl}(\theta) \) for finding the wave function by formula (2).

From the wave function we found the tunneling current density inside the barrier including scatterer. The spatial distribution of \( j \) and \( j_y \) components of the current which flow from left side of the barrier (\( z = z_{left} = -0.02 \mu \)) to the right side (\( z = z_{right} = +0.02 \mu \)) are shown in figures 3-6. These figures demonstrate the nonuniform character of the current density. The scatterer is located in the position \( z = 0 \) and \( y = 0 \). The figures 3, 4 correspond to the attractive case: \( V_s < V_b \) where \( V_s \) is the potential of scatterer and \( V_b \) is the barrier potential. In this case the current flows mainly through the scatterer and its surrounding region. Thus the scatterer forms an additional channel for current. The figures 5, 6 correspond to the repulsive case: \( V_s > V_b \). In this case the current flows mainly far away from the scatterer and penetration of the barrier decreases. It also means that the leakage current to the scatterer is small enough and it is possible to control the total current through barrier by the change of scatterer potential with small power.
Figure 3. Distribution of the current $J_z$ in the barrier when $V_s$ is less than $V_b$.

Figure 4. Distribution of the current $J_y$ in the barrier when $V_s$ is less than $V_b$.

Figure 5. Distribution of the current $J_z$ in the barrier when $V_s$ exceed $V_b$.

Figure 6. Distribution of the current $J_y$ in the barrier when $V_s$ exceed $V_b$.

In summary, we have developed the algorithm for computer simulation of under barrier transport of electrons through the nonuniform semiconductor barriers containing nanometer scatterers. The scatterers may have spherical or cylindrical shapes with radial dependent potential. The results of simulation of the tunneling current density in the non uniform barrier demonstrate the possibility of the current control by the external potential applied to embedded scatterers, especially for cylindrical shape. These results hold promise for the development of new types of active devices with embedded quantum wires into the barrier, like a grid in the vacuum triode. It is also shown that the tunneling through Gamow window produce the population inversion of transmitted carriers.

References
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