Calculation of current-voltage characteristic of a resonant-tunneling diode (RTD) and using the adiabatic approximation for simulation of conductance quantization in quantum point contact (QPC)

P. Wójcik, A. Mreńca-Kolasińska

January 29, 2025; last updated February 14, 2025

1 Wstęp

This task consists of two parts, considering transport simulation in two nanodevices:

- resonant-tunneling diode,
- quantum point contact in a 2D nanowire, within the adiabatic approximation.

Both methods are based on calculations of the transmission coefficient, which describes the probability of an electron incident in the left contact will leave the device through the right contact. The transmission coefficient calculations here are done with the 1D transfer matrix method.

2 Transfer matrix method

Consider the Schrödinger equation for a 1D open system, with a position-dependent electron mass

$$-\frac{\hbar^2}{2}\frac{d}{dz}\frac{1}{m^*(z)}\frac{d}{dz}\psi(z) + U(z)\psi(z) = E\psi(z), \tag{1}$$

where $m^*(z)$ describes the effective mass at position z, and $U(z)$ is the potential energy profile. We divide the nanodevice area $[0, L]$ into N parts so small, that in each interval $[z_{n-1}, z_n]$ the potential $U(z)$ and electron mass $m^*(z)$ can be assumed constant. The Schrödinger equation in the interval $[z_{n-1}, z_n]$ is

$$-\frac{\hbar^2}{2m_n^*}\frac{d^2}{dz^2}\psi_n(z) + U_n\psi_n(z) = E\psi_n(z), \tag{2}$$

and its solution in this interval is the wave function

$$\psi_n(z) = A_n e^{ik_n z} + B_n e^{-ik_n z}, \tag{3}$$

where

$$k_n = \frac{1}{\hbar}\sqrt{2m_n^*(E - U_n)}, \tag{4}$$

and A_n and B_n are amplitudes of the plane wave propagating to the right and left, respectively.
Notice that the wave function at the border of each interval needs to be continuous, thus

$$\psi_n(z_n) = \psi_{n+1}(z_n). \tag{5}$$

The probability density flux also needs to be continuous

$$j_n = j_z(z_n) = \frac{i\hbar}{2m_n}\left[\psi(z_n)\frac{d\psi^*(z)}{dz}\bigg|_{z=z_n} - \psi^*(z_n)\frac{d\psi(z)}{dz}\bigg|_{z=z_n}\right], \tag{6}$$

which leads to the continuity condition

$$\frac{1}{m_n}\frac{d}{dz}\psi_n(z_n) = \frac{1}{m_{n+1}}\frac{d}{dz}\psi_{n+1}(z_n). \tag{7}$$

Applying the continuity conditions between intervals $[z_{n-1}, z_n]$ and $[z_n, z_{n+1}]$, we get

$$\begin{pmatrix} A_n \\ B_n \end{pmatrix} = \mathcal{M}_n \begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix}, \tag{8}$$

where the matrix $\mathcal{M}_n$ is called monodromy matrix. It is a square matrix, the elements of which are:

$$\begin{aligned}
\mathcal{M}_{n,11} &= \frac{1}{2}\left(1 + \frac{k_{n+1}m_n^*}{k_n m_{n+1}^*}\right)\exp\left(i(k_{n+1} - k_n)z_n\right), \\
\mathcal{M}_{n,12} &= \frac{1}{2}\left(1 - \frac{k_{n+1}m_n^*}{k_n m_{n+1}^*}\right)\exp\left(-i(k_{n+1} + k_n)z_n\right), \\
\mathcal{M}_{n,21} &= \frac{1}{2}\left(1 - \frac{k_{n+1}m_n^*}{k_n m_{n+1}^*}\right)\exp\left(i(k_{n+1} + k_n)z_n\right), \\
\mathcal{M}_{n,22} &= \frac{1}{2}\left(1 + \frac{k_{n+1}m_n^*}{k_n m_{n+1}^*}\right)\exp\left(-i(k_{n+1} - k_n)z_n\right).
\end{aligned} \tag{9}$$

Applying the monodromy matrix sequentially between all intervals we get

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \mathcal{M}_{1\to N} \begin{pmatrix} A_N \\ B_N \end{pmatrix}, \tag{10}$$

where

$$\mathcal{M}_{1\to N} = \mathcal{M}_1\mathcal{M}_2\ldots\mathcal{M}_{N-1}. \tag{11}$$

Notice that in the rightmost interval there are no backscattered electrons, so $B_N = 0$. Then the transmission and reflection coefficients are given by the formulas

$$T = \frac{k_N m_1}{k_1 m_N}\frac{|A_N|^2}{|A_1|^2}, \tag{12}$$

$$R = \frac{|B_1|^2}{|A_1|^2}. \tag{13}$$

$$\tag{14}$$

Additionally, assuming $A_N = 1$, we get

$$T = \frac{k_N m_1}{k_1 m_N}\frac{1}{|\mathcal{M}_{1\to N,11}|^2}, \tag{15}$$

$$R = \frac{|\mathcal{M}_{1\to N,21}|^2}{|\mathcal{M}_{1\to N,11}|^2}. \tag{16}$$

$$\tag{17}$$

In the calculations, we will change the energy of the incident electron and get two quantities $R(E)$ and $T(E)$ that satisfy $T(E) + R(E) = 1$.

2.1 Tasks

Consider the device shown in Fig. 1. Since the band gap in GaAs is different than the band gap in AlGaAs, the potential that the electron "sees" has the shape of a single potential barrier shown in the figure.

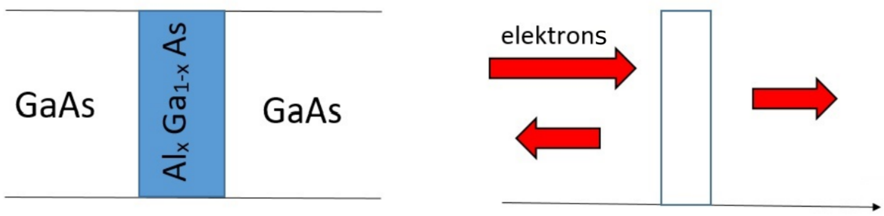

Figure 1: Schematic of the GaAs/$Al_{0.3}Ga_{0.7}$As tunnel structure with the effective potential felt by the electron flowing through the nanodevice.

Let us consider the following parameters of the device: the width of the AlGaAs layer $d_{AlGaAs} = 5$ nm, effective mass in the materials $m^*_{GaAs} = 0.063m_0$ for GaAs, and $m^*_{AlGaAs} = (0.063+0.083x)m_0$ for $Al_xGa_{1-x}As$. Perform the calculations for $x = 0.3$, and barrier height $U = 0.27$ eV.

1. Calculate the transmission and reflection coefficients of the device as a function of energy, assuming constant effective mass in the nanodevice $m^* = m^*_{GaAs} = 0.063$. Compare the numerical results with analytical transmission coefficient values[1].

2. Calculate the transmission and reflection coefficients assuming spatially varying effective mass, different in GaAs and AlGaAs.

3 Resonant-tunneling diode

Resonant-tunneling diode is a planar electronic device characterized by nonlinear current–voltage behavior, with the distinctive region of negative differential resistance – see Fig. 2

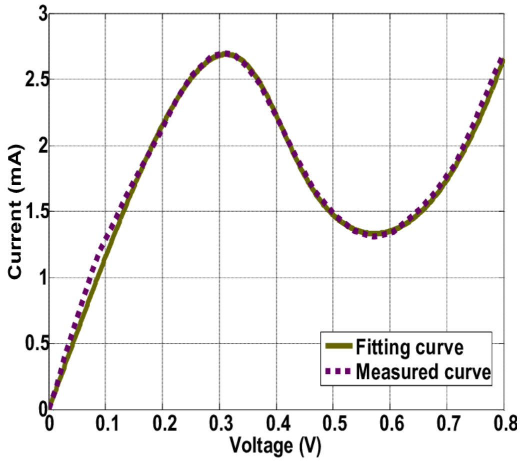

Figure 2: Current–voltage characteristic of RTD with the distinctive region of negative differential resistance (NDR).

A typical RTD structure is shown in Fig. 3. Assuming the semiconductor structure as in Fig. 3, we can assume that the potential profile in the nanodevice is a double barrier-like potential.

Figure 3: Schematic of the RTD strukture based on $GaAs/Al_{0.3}Ga_{0.7}As$, and the effective potential felt by the electron flowing through the nanodevice.

In our calculations, we will assume space-dependent effective mass $m^*_{GaAs} = 0.063m_0$ in GaAs, and $m^*_{AlGaAs} = (0.063+0.083x)m_0$ in $Al_xGa_{1-x}As$. Perform the calculations for $x = 0.3$, and barrier height $U = 0.27$ eV, barrier width $d_{AlGaAs} = 5$ nm, and quantum well width $d_{GaAs} = 3$ nm.

3.1 Tasks

1. Using the transfer matrix method implemented earlier, calculate the transmission and reflection coefficients of the considered device. What distinctive feature of quantum transport can you see in the $T(E)$ plot?

[1] See e.g. Sakurai, appendix B.3.

2. Calulate current–voltage characteristic of the RTD diode using the Tsu-Esaki formula

$$j = \frac{em^* k_B T}{2\pi^2 \hbar^2} \int_0^\infty dE_z T(E_z) \ln \left[\frac{1 + e^{(\mu_s - E_z)/k_B T}}{1 + e^{(\mu_d - eV_{bias} - E_z)/k_B T}} \right], \tag{18}$$

where $\mu_{s,d}$ is the chemical potential of the source and drain, V_{bias} is the applied voltage, and T is temperature. Assume $\mu_s = \mu_d = 87$ meV and $T = 77$ K. Remember that applying bias voltage in the device is also associated with a linear decrease in potential in the nanostructure, as shown in Fig. 4.

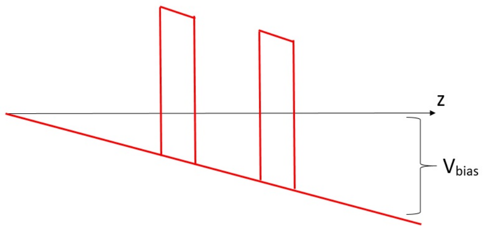

Figure 4: linear decrease of potential resulting from the voltage V_{bias} applied to RTD diode.

4 Quantum point contact in the adiabatic approximation – conductance quantization

Consider a quantum point contact (QPC) defined in the two dimensional electron gas (2DEG) – see Fig. 5.

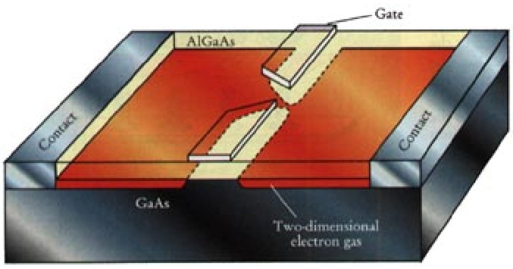

Figure 5: Qquantum point contact based on 2DEG.

Potential induced in the system by the applied gate voltage V_g can be described by the formula

$$V(x, y) = f[x - l, y - b] + f[x - l, t - y] + f[r - x, y - b] + f[r - x, t - y], \tag{19}$$

where

$$f(u, v) = \frac{eV_g}{2\pi\varepsilon} \tan^{-1} \left(\frac{uv}{d\sqrt{d^2 + u^2 + v^2}} \right), \tag{20}$$

where ε is the permittivity of the material, l, r are the positions of the left and right edge of the gate, t and b are the positions of the gate edges in the vertical direction, and d is the distance between the gates and 2DEG. In general, this is a 2D device, described by the Schrödinger equation

$$-\frac{\hbar^2}{2m^*} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \psi(x, y) + V(x, y)\psi(x, y) = E\psi(x, y). \tag{21}$$

The adiabatic approximation assumes that the change of the potential in the x direction is much slower than in the transverse y direction. Then we can assume

$$\psi(x, y) = \sum_n \phi_n(x)\chi_n(y; x) \tag{22}$$

where $\chi(y;x)$ means that χ is a function of the variable y with a constant parameter x.
With this assumption, the Schrödinger equation can be separated into two equations (details in the lecture)

$$-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial y^2}\chi_n(y) + V(y;x)\chi_n(y;x) = E_n\chi_n(y;x), \quad (23)$$

$$\left[-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial x^2} + E_n(x)\right]\phi_n(x) = E\phi_n(x). \quad (24)$$

Investigation of the electron transport through this system is based on solving the second of these equations for the potential $E_n(x)$, where $n = 1, 2, 3, \ldots$, obtained from the diagonalization of the first equation for the given parametrs x.

In the calculations, assume the following values of the material parameters: effective mass $m^*_{GaAs} = 0.063$, dielectric constant $\varepsilon = 13.6$ width of the 2DEG $W = 50$ nm, length $L = 100$ nm, position of the QPC gates in the range $[0.3, 0.7]L$ with the spacing between the gates $0.6W$, $d = 3$ nm, and $V_g = 4$ eV.

4.1 Tasks

1. Plot the effective potential felt by the electron flowing through the QPC, i.e. $E_n(x)$, for $n = 1, 2, 3, \ldots$
2. Using the Landauer formula calculate conductance as a function of the incident electronu energy $G(E)$, with

   $$G = \frac{2e^2}{h}\sum_n T_n(E). \quad (25)$$

   Use the transfer matrix method to calculate $T(E)$.
3. Using the Landauer formula calculate conductance as a function of the gate voltage, for two values of Fermi energy: $E = 50$ meV and $E = 100$ meV.