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Resonant tunnelling of electrons in multi-step single-barrier heterostructures*

Wang Chang(王 长)† and Zhang Yong-Hua(张拥华)

State Key Laboratory of Functional Materials for Informatics, Shanghai Institute of Microsystem and Information Technology, Chinese Academy of Sciences and Graduate School of Chinese Academy of Sciences, Shanghai 200050, China

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We have studied the quantum transport of electrons in a three-step single-barrier AlGaAs heterostructure under electric field. Using the quantum transmitting boundary method and Tsu–Esaki approach, we have calculated the transmission coefficient and current–voltage characteristic. The difference of the effective mass among the three barriers is taken into account. Effects of the barrier width on transmission coefficient and peak-to-valley current ratios are examined. The largest peak-to-valley current ratio is obtained when the ratio of widths of the left, middle, and right barrier is fixed at 4:2:1. The calculated results may be helpful for designing devices based on three-step barrier heterostructures.

Keywords: electron transport, heterostructure, resonant tunnelling, AlGaAs
PACC: 7200, 7300, 7335C, 7360P

1. Introduction

Since the pioneering work of Tsu and Esaki,[1] electron transport in resonant tunnelling heterostructures has been an active field, and has attracted a great deal of attention both theoretically and experimentally over the past 20 years.[2−22] The large amount of research in this field is sparked by new technical advances in nano-fabrication and new potential applications, such as terahertz optoelectronic devices.[9,23−27] In resonant tunnelling structures, the transmission coefficient (TC) is one of the most useful parameters to understand the resonant tunnelling phenomenon. Generally, the value of TC is suppressed when an electric field is applied to the symmetrical rectangular multibarrier heterostructures. While for asymmetrical multibarrier structures, the effect of voltage on TC is very complicated. It is shown that for appropriate choices of asymmetry in the barrier widths and heights of the heterostructure, the TC is enhanced to yield resonances that are stronger than those calculated in symmetric structures.[10] The TCs in most of the theoretical works are calculated using the transfer matrix method, analytical approach with Airy function,[15] or difference equation approach.[16] It is worth noting that the difference equation approach is numerical stable and can be applied to treat hole tunnelling and interband tunnelling.

Step-barrier structure, first proposed by Schulz and Gonçalves da Silva,[4] is a unique structure that breaks the symmetrical behaviour under positive or negative dc voltage bias shown by double-barrier quantum well diode. The TC of the two-step barrier structure under the influence of dc voltage was numerically calculated by taking into account the coupling between components of the motion of an electron in directions parallel and perpendicular to the interfaces.[17] It is shown that the global behaviour of the step-barrier structure resembles the asymmetric double-barrier structures.[17] The peak-to-valley current ratios of the structure are much larger than those for the single-barrier structure. The experimental observation of negative differential resistance at room temperature in a three-step single-barrier AlGaAs structure is recently reported by Emellet *et al.*[19] In their work, the TC of the structure is obtained using the commercial software. The measured current–voltage characteristic has a peak-to-valley ratio larger than unity.

Despite the practical interest in three-step bar-

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†Corresponding author. E-mail: cwang@mail.sim.ac.cn

rier structure, there has no theoretical investigation on electron transport in the structure. Here, we explicitly consider the electron transport in a AlGaAs-based three-step single-barrier structure under the influence of dc voltage bias, using the quantum transmitting boundary method (QTBM). QTBM is robust and numerically stable as compared to the transfer matrix method, which is usually used in calculating TC of resonant tunnelling structures. The effect of the voltage bias and the size of the three-step single-barrier structure on TC and current–voltage (I–V) characteristic are discussed. The results show that a proper choice of voltage bias can lead to complete transmission in the step-barrier structure. The largest peak-to-valley current ratio is also obtained by changing the width of the barriers.

2. Tunnelling model and theory

The one-dimensional schematic energy diagram of the three-step single-barrier structure is depicted in Fig.1, where E_{F} is the Fermi level of the GaAs contact. U_1 and b_1 are the height and width of the left barrier, U_2 and b_2 are those for the middle one, and U_3 and b_3 are those for the right one, respectively. The

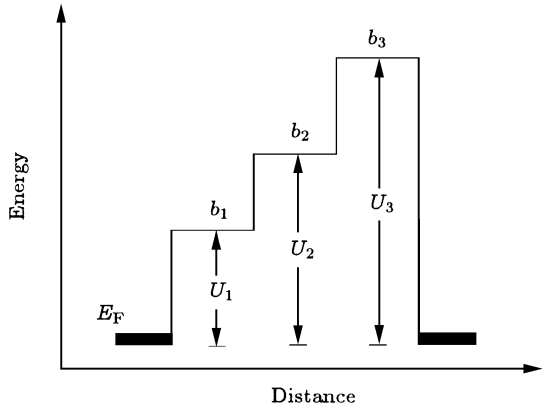


Fig.1. Conduction-band edge of the three-step single-barrier heterostructure without voltage bias.

total width of the step-barrier structure is $b = b_1 + b_2 + b_3$. We consider that the electron with energy E is incident from the left contact region and transmits to the right one across the energy barrier. Within the effective mass approximation, this process can be described by the one-dimensional Schrödinger equation

$$-\frac{\hbar^2}{2}\frac{\mathrm{d}}{\mathrm{d}z}\left(\frac{1}{m(z)}\frac{\mathrm{d}}{\mathrm{d}z}\psi(z)\right)+V(z)\psi(z)=E\psi(z), \quad (1)$$

where the z axis represents the growth direction of the structure, $m(z)$ is the space dependent electron effective mass, $V(z)$ includes both the band-edge discontinuities and macroscopic electric fields, and $\psi(z)$ is the wave function. The effective mass Schrödinger equation (1) can be described using the finite difference method and expressed as

$$H_{i,i-1}\psi_{i-1}+\bar{H}_{i,i}\psi_i+H_{i,i+1}\psi_{i+1}=0, \quad (2)$$

where

$$H_{i,i\pm1}=-\frac{\hbar^2}{d^2}\left(\frac{1}{m_i+m_{i\pm1}}\right), \quad (3)$$

$$H_{i,i}=V_i-H_{i,i+1}-H_{i,i-1}, \quad (4)$$

and $\bar{H}=H-E$, with d being the space between the mesh points and i the discretization index ($1<i<N$, N being the number of mesh points).

We use the QTBM to describe the boundary conditions. The QTBM was first proposed by Lent and Kirkner[28] for treating electron waveguides, and adapted by Frensley[29] to treat heterostructure tunnelling devices. Ting[30] extended the QTBM to treat the multiband model and obtain stable and efficient solutions when calculating TCs in heterostructures. Recently, Lü and Cao[31] studied the ballistic tunnel injection transit-time diode using the single-band QTBM and obtain interesting results. Here, we closely follow their suggestion. Assuming that the electron is moving from the left lead to the right lead, we have the boundary conditions at the left and right regions which are considered as semi-infinite flat-band, respectively,[31]

$$\psi(1)-\mathrm{e}^{\mathrm{i}k_{\mathrm{L}}d}\psi(2)=a_{\mathrm{L}}\left(1-\mathrm{e}^{2\mathrm{i}k_{\mathrm{L}}d}\right), \quad (5)$$

$$\psi(N)-\mathrm{e}^{\mathrm{i}k_{\mathrm{R}}d}\psi(N-1)=a_{\mathrm{R}}\left(1-\mathrm{e}^{2\mathrm{i}k_{\mathrm{R}}d}\right), \quad (6)$$

where k_{L} and k_{R} are the wave numbers of the left and right boundary regions, respectively, a_{L} and a_{R} are the amplitudes of the incoming wave components in the left lead and right leads, respectively (for detail, see Ref.[29]). In our calculation, a_{R} is set to be zero since there exist no wave components coming into the barrier from the right lead. The two boundary conditions together with Eq.(2) constitute a tri-diagonal system of N linear equations with N unknowns $\psi(1)$, $\psi(2)$,..., $\psi(N)$, which can be numerically solved with the available routines. The TC of the structure can be given by

$$T=\frac{k_{\mathrm{R}}}{k_{\mathrm{L}}}\left|\psi(N-1)\right|^2. \quad (7)$$

It is evident that the TC of the structure is determined by the electron incident energy E and the external applied voltage V_{a}.

With the calculated TC of the structure, the current density can be obtained easily by the Tsu-Esaki equation[1]

$$J = \frac{em_0^* k_B T}{2\pi^2 \hbar^3} \int_0^\infty T(E) \times \ln\left[\frac{1+\exp\left[(E_F - E)/(k_B T)\right]}{1+\exp\left[(E_F - eV_a - E)/(k_B T)\right]}\right] dE, \quad (8)$$

where V_a is the applied voltage, the quantities E, m_0^*, k_B, T, and $\hbar$ are the electron incident energy, electron effective mass, Boltzmann's constant, absolute temperature, and Planck's constant, respectively.

3. Simulation results and discussion

In this section, we carry out the numerical simulation of TC and current density of the three-step single-barrier structure under an applied voltage. Different barrier heights can be obtained by changing the concentration of aluminium. In our calculation, the aluminium concentrations are set at 0.15, 0.25, and 0.35 in the left, middle, and right barriers, respectively. We first calculated the TCs for electron tunnelling through the step-barrier structure for different voltage biases, as depicted in Fig.2. The widths of the three barriers are set as $b_1 = b_2 = b_3$=30Å. It is shown that TC at V_a=0 is under unity and no transmission resonance (or optimal resonant tunnelling) occurs. With the increase of the applied voltage, transmission resonances appear for some specific voltage biases (such as V_a=0.2 V and V_a=0.62 V in Fig.2). This is different from the case for single-barrier structure or symmetric double- or triple-barrier structures, where the resonance peaks will be suppressed with the increase of voltage bias. The appearance of transmission resonances for specific voltages is mainly due to the enhancement of symmetry of the heterostructures under positive bias. It is observed that the resonant peak in the case of V_a=0.62 V is much narrower than that for V_a=0.2 V, while the TC for V_a=0.93 V is suppressed and the peak are broadened and shifted to the lower-energy region. The transmission coefficient for V_a=0.62 V is enhanced drastically at the outset and a complete transmission resonance is produced at the energy E=0.1112 eV. This can be due to the formation of wells with triangular shape when the voltage bias is applied.[4] The occurrence of unity transmission at specific values of the voltage bias in the three-step barrier structure is different from that of the two-step barrier one, where transmission resonance can be obtained for every positive bias voltages.[17]

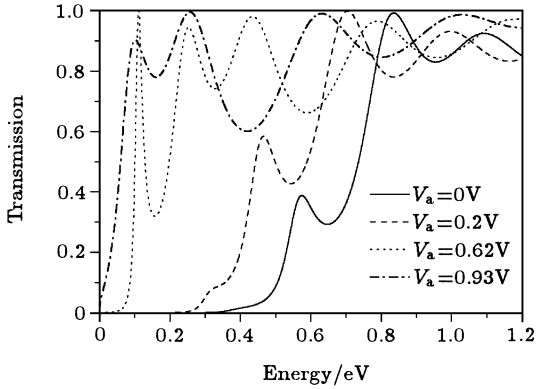


Fig.2. Transmission coefficient of the electron tunnelling through the three-step barrier structure as a function of electron energy at voltages V_a=0, 0.2, 0.62, and 0.93 V, respectively. The widths of the three barriers are $b_1 = b_2 = b_3$=30Å.

To have a deep insight into the characteristic of resonant tunnelling, we have calculated the TC by changing the width of the step-barrier structure. The widths b_1, b_2, and b_3 of the three barriers are set as 20, 20, and 20Å(a), 20, 20, and 40Å(b), 20, 40, and 20Å(c), and 40, 20, and 20Å(d). The TCs of these structures without voltage bias are depicted in Fig.3. It is shown that more peaks show up in the curve with the increase of the total barrier width b. Comparing the result of (a) with (b), (c), and (d), one can see that the width of resonant peaks get narrower with the increase of total barrier width. In (b), (c), and (d) which have the same total barrier width b, it is found that with the thicker barrier shifted from the right barrier to the left one, the widths of the resonant peaks are broadened. From Fig.3, we observe that complete resonant tunnelling occurs above the effective-potential height. This is caused by the appearance of quasi-bound states above the barrier at zero bias, which has been demonstrated experimentally by Luo *et al*[32] in a single-barrier structure.

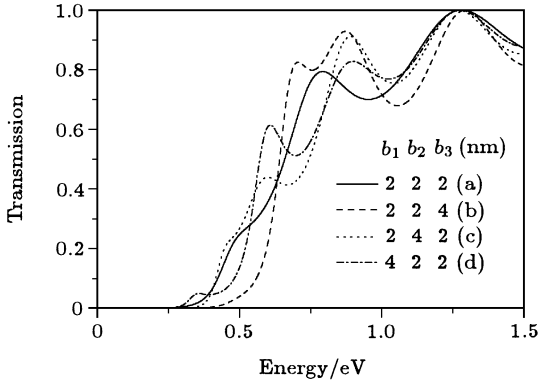


Fig.3. Transmission coefficients of the three-step single-barrier structure for different barrier width b. The widths of b_1, b_2, and b_3 are set at 20, 20, and 20Å(a), 20, 20, and 40Å(b), 20, 40, and 20Å(c), and 40, 20, and 20Å(d), respectively.

The I–V characteristic is an important parameter for designing devices based on the resonant tunnelling structure. We have calculated the current density of the three-step single-barrier structure with total barrier width b=63Å(a) and b=84Å(b) when temperature $T \to 0$ K. In our calculation, the Fermi level is fixed at 10 meV and the ratio of the widths of the left, middle, and right barrier are set at 1:1:1 (i), 1:2:4 (ii), and 4:2:1 (iii). The calculated current density is depicted in Fig.4. One can easily see that there are several current peaks in each of the current–voltage curves and more peaks show up with the increase of total barrier width b. Sharp current peaks and large peak-to-valley current ratios show up at low voltage bias in the cases (i) and (iii) in Figs.4(a) and 4(b), respectively. Several negative differential resistance regions are observed following the sharp current peak. While in the case (ii) in Figs.4(a) and 4(b), the first current peak increases very slowly and then a negative differential resistance region also appears. From Figs.4(a) and 4(b), the largest peak-to-valley current ratio shows up when the ratio of the three barriers is fixed at 4:2:1 (iii), which agrees, at least in principle, with the prediction of Guo *et al.*[17] From the application point of view, large peak-to-valley current ratio of heterostructures is of importance for high-frequency optoelectronic device application. It is found that the largest peak-to-valley current ratios of the three-step barrier structure are 4.87 for b=63Å and 7.54 for b=84Å. The peak-to-valley current ratio of the three-step barrier structure is much larger than that of the two-step one, which is only 1.82. The experimentally measured peak-to-valley current ratio of the three-step barrier structure is only 1.05 at 300 K.[19] The calculated results also indicate that large peak-to-valley current ratio can be obtained by the proper choice of the total width of the three-step barrier structure.

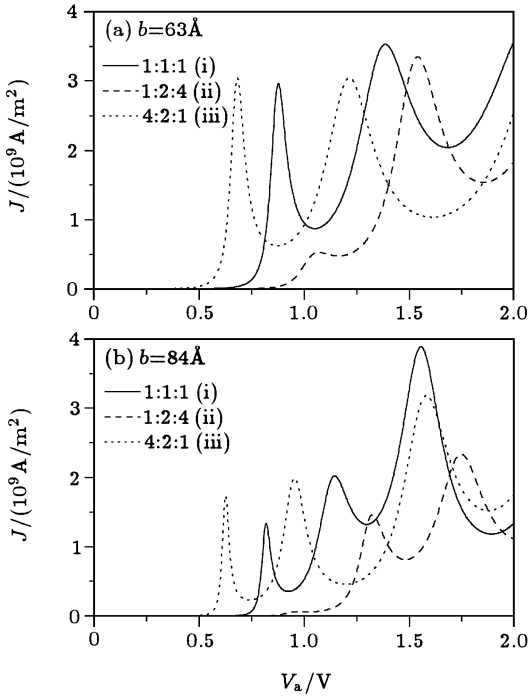


Fig.4. I–V characteristic of the three-step single-barrier structure with the total width b=63Å(a) and b=84Å(b) as $T \to 0$ K. The ratios of the width of the three parts of the barrier are set to be 1:1:1 (i), 1:2:4 (ii), and 4:2:1 (iii), respectively.

4. Conclusions

We have theoretically studied electron resonant tunnelling in a three-step single-barrier structure with or without voltage bias using the QTBM. With the influence of dc voltage bias, the degree of symmetry is enhanced and complete resonant tunnelling can be obtained for some specific voltage bias. If the voltage bias is further increased, the degree of symmetry may be lowered and complete resonant tunnelling will disappear. Thus complete resonant tunnelling can be obtained by the proper choice of the voltage bias. The I–V characteristics are calculated by changing the total barrier width and the ratio of the left, middle, and right barrier widths. Largest peak-to-valley current ratio can be obtained when b_1:b_2:b_3 is fixed at 4:2:1.

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