Journal of The Islamic of Gaza(Natural Sciences Series) Vol.13, No.2, P203-211, 2005
ISSN 1726-6807, http://www.iugaza.edu/ara/research/

ELECTRONIC TRANSMISSION THROUGH QUANTUM WIER CONTAINING HETERO-JUNCTIONS

H. M. Fayad, [1] and M. M. Shabat [2]
[1] Physics Department, Al-Aqsa University, Gaza, Gaza Strip, Palestine.
[2] Physics Department, The Islamic University, Gaza, P. O. Box 108, Gaza Strip, Palestine.

Abstract: By means of mode-matching and transfer matrix methods, we calculate the transmission of an electron passing through quantum wire consisting of several barrier potentials. We take into account the space-dependent electron effective mass and the coupling between components of the motion of an electron in directions parallel and perpendicular to the interfaces of barriers. Our results show that the coupling effect leads to significant changes on the transmission spectra. In addition, the variation of the geometrical dimensions is investigated.

***Keywords*:** Quantum transport; Mesoscopic systems; Electron waveguides

1. INTODUCTION

With the rapid progress in nanofabrication technology, semiconducting nanowires have been extensively studied for the potential applications on nanoelectronics. Tsu and Esaki [1] realized the theoretical significance of the resonant-tunneling problem in semiconductor heterostructure. Double-barrier resonant-tunneling structures have found wide applications in many new devices, such as photo-detectors, diodes, transistors, low-power logic circuits, and quantum integrated circuits [2,3]. There mainly exist two theoretical frameworks for dealing with resonant tunneling problems. One is the tight-binding model [4,5]. The other is the parabolic-band effective-mass approximation, in which, the coherent tunneling model [6] and the sequential tunneling model [7] have been proposed and developed for investigating resonant-tunneling characteristics in multibarrier heterostructure [8]. In the coherent tunneling model, an electron keeps its phase memory in the tunneling process, which is regarded as a coherent transmission process and described by the eigenstate of the electron in the total structure. In the sequential tunneling model, the electron loses its phase memory in the tunneling process, which is regarded as a series of successive transition processes with phase incoherence. The effective-mass approximation is restricted to the assumption that the components of the motion of the electron in the directions normal and parallel to the layers are decoupled. However, this assumption is incorrect when the difference of the effective mass of the electron in the barrier and well materials is taken into account. It arises because of the following reason. When the effective mass is space dependent, the conservation of momentum of the electron in the parallel direction does not imply conservation of the kinetic energy component in the direction parallel to the layers. As a result less or more energy is available for the motion perpendicular to the barrier, which hinders or helps the tunneling process.

With the molecular-beam-epitaxy technology, it is possible to construct two-dimensional barrier structures such as GaAs-GaAlAs-GaAs in which the width of each layer is controlled with considerable accuracy. The effective mass of the electron in such a structure is position dependent as a consequence of its value changing in GaAlAs as a function of aluminum concentration while remaining constant in GaAs. As shown by Lee [9], the effective mass difference in the two layers is sufficient to bring about significant changes in the tunnel time and transmission coefficient.

In this paper, we explore the effect of coupling between the parallel motion and the normal motion of the electron on resonant-tunneling characteristics in quantum wire containing multi-barrier heterostructure (section 2). With the transfer matrix method, the electronic transmission through the proposed quantum wire is discussed (section 3).

2. TRANSFER MATRIX METHED OF QUANTUM WIRE

We consider a double barrier heterostructure (one segment of our quantum wire) consisting of AlAs (barrier layers) and GaAs (well layer) as shown in Fig. 1.

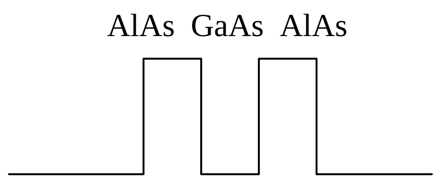

Fig.1. Schematic illustration of a double barrier heterostructure.

Let us consider a beam of electrons with kinetic energy E and effective mass m to be incident on a barrier from the left. We describe the problem using the parabolic-band effective-mass approximation. Because of the spatial symmetry in all directions parallel to the layers, the wave vector $k_o = (k_y, k_z)$ of the electron is conserved in the y-z plane and the corresponding electron wave function is expressed by a plane wave. The total wave function $\psi(r, x)$ for the electron can be written as

$$\psi(r,x) = \exp(ik_o r)\varphi(x) \qquad (1)$$

where $\varphi(x)$ satisfies the one-dimensional (1D) Schrödinger equation with position-dependent electron effective mass, x represents the growth direction of heterostructure, and $r = (y,z)$ is the position coordinate of the electron in the plane of the barrier.
The 1D Schrödinger equations are

$$\frac{-\hbar^2}{2m_w(x)}\frac{d^2\varphi(x)}{dx^2} = E_x^w\varphi(x) \qquad (2)$$

in the well region, and

$$\frac{-\hbar^2}{2m_b(x)}\frac{d^2\varphi(x)}{dx^2} + U_o\varphi(x) = E_x^b\varphi(x) \qquad (3)$$

in the barrier region, where $E_x^w = E - E_o^w$ and $E_x^b = E - E_o^b$ are the longitudinal energies of the electron in the well and barrier, respectively, $m_w(x)$ and $m_b(x)$ are the position-dependent electron effective mass in the well and barrier, respectively. Here $E_o^w = \frac{\hbar^2 k_o^2}{2m_w}$ and $E_o^b = \frac{\hbar^2 k_o^2}{2m_b}$ are, respectively, the transverse kinetic energy of the electron in the well and the barrier. Thus it can be seen that the position-dependent electron effective mass effects the wave function $\varphi(x)$ and introduces a coupling between the wave function in the parallel and perpendicular directions. As a consequence the wave function $\varphi(x)$ is influenced not only by the width (b) and the barrier height (U_o) but also by the wave vector k_o of the plane wave parallel to the layers. Accordingly, we introduce an effective barrier height $U(k_o)$ for tunneling of electrons along the x-direction as [10]

$$U(k_o) = U_o - (1-\beta)\frac{\hbar^2 k_o^2}{2m_w(x)} \qquad (4)$$

where $\beta = \frac{m_w}{m_b}$. Taking into account Eq. (4), the 1D Schrödinger equation in the barrier region becomes:

$$\frac{-\hbar^2}{2m_b(x)}\frac{d^2\varphi(x)}{dx^2}+U(k_o)\varphi(x)=E_x^w\varphi(x) \qquad (5)$$

Thus, the coupling can be interpreted as meaning that the effective barrier height “felt” by the electron is no longer a constant U_o.

Now, we need the transfer matrix for the *j*th junction, and then we should generalize the result for *N*-junctions. This matrix relates the coefficients of the wave function at one end of the junction to those at the other one, so that, the wave functions are written as

$$\varphi_j^w(x)=A_j^w\exp(ik_x x)+B_j^w\exp(-ik_x x) \qquad (6)$$

for the *j*th well, and

$$\varphi_j^b(x)=A_j^b\exp(k_b x)+B_j^b\exp(-k_b x) \qquad (7)$$

for the *j*th barrier

where $k_x=(2m_w(x)E_x/\hbar^2)^{1/2}$, $k_b=\left[2m_b(x)(U(k_o)-E_x)/\hbar^2\right]^{1/2}$, and E_x is the longitudinal kinetic energy of the incident electron.

By matching the continuity of the wave function $\varphi(x)$ and its appropriately normalized derivative $\frac{1}{m(x)}\frac{d\varphi(x)}{dx}$ at the boundaries, we derive a matrix formula that relates the coefficients A_j^w and B_j^w with A_{j+1}^w and B_{j+1}^w, that is:

$$\begin{pmatrix}A_j\\B_j\end{pmatrix}=\frac{1}{2}\begin{pmatrix}1 & -ik_x^{-1}\\1 & ik_x^{-1}\end{pmatrix}M_j\begin{pmatrix}1 & 1\\ik_x & -ik_x\end{pmatrix}\begin{pmatrix}A_{j+1}\\B_{j+1}\end{pmatrix} \qquad (8)$$

where M_j is the *j*th transfer matrix corresponding to the *j*th junction written as:

$$M_j=M_b(b_j)M_w(a_j)M_b(b_{j+1}) \qquad (9)$$

where b_j and a_j are the widths of the *j*th barrier and *j*th well, respectively, $M_b(b_j)$ and $M_w(a_j)$ correspond to the transfer matrices for the *j*th barrier and *j*th well respectively,

$$M_b(b_j) = \begin{pmatrix} \cosh(k_b b_j) & -(\beta k_b)^{-1}\sinh(k_b b_j) \\ -\beta k_b \sinh(k_b b_j) & \cosh(k_b b_j) \end{pmatrix} \qquad (10)$$

and

$$M_w(a_j) = \begin{pmatrix} \cos(k_x a_j) & -(k_x)^{-1}\sin(k_x a_j) \\ -k_x \sin(k_x a_j) & \cos(k_x a_j) \end{pmatrix} \qquad (11)$$

Setting $A_1 = 1$, $B_1 = r$, $A_N = t$, and $B_N = 0$, then the total transfer matrix is expressed as the cascading of a series of the individual barrier and well transfer matrices in sequence

$$\begin{pmatrix} 1 \\ r \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & -ik_x^{-1} \\ 1 & ik_x^{-1} \end{pmatrix} M_{tot} \begin{pmatrix} 1 & 1 \\ ik_x & -ik_x \end{pmatrix}\begin{pmatrix} t \\ 0 \end{pmatrix} \qquad (12)$$

with

$$M_{tot} = \left[\prod_{j=1}^{N-1} M_b(b_j) M_w(a_j)\right] M_b(b_N) \qquad (13)$$

From Eq. (12), it is readily found that the transmission amplitude t is given by

$$t = \frac{2}{M_{11} + M_{22} + i(k_x M_{12} - k_x^{-1} M_{21})} \qquad (14)$$

where M_{ij} is the elements of the total transfer matrix. Thus, the transmission coefficient T is now defined as the ratio of the transmitted particle flux divided by incident particle flux, and depends upon both the transfer wave number and the longitudinal kinetic energy of the incident electron. This definition leads directly to the following expression:

$$T(k_o, E_x) = |t|^2 \qquad (15)$$

3. RESULTS AND DISCUSSION

In this section we present our results obtained numerically for the transmission coefficient across the quantum wire containing multi-barrier heterostructure consisting of $GaAs/Ga_{1-z}Al_zAs$, where z represents the concentration of Al. In this structure the conduction-band offset and the effective mass of the electron are determined as a function of the Al concentration *z* by the following standard approximation [11]

$$U_o = \begin{cases} 0.75z \quad (eV) & (0 \prec z \le 0.45) \\ 0.75z + 0.69(z-0.45)^2 \;\; (eV) & (0.45 \le z \le 1) \end{cases} \tag{16}$$

and

$$\begin{aligned} m_b &= (0.067 + 0.083z)m_e \qquad (0 \prec z \le 1), \\ m_w &= 0.067 m_e \end{aligned} \tag{17}$$

where m_e is the free-electron mass.

The dependence of the transmission coefficient *T* on the longitudinal kinetic energy and the transverse wave number of the electron is shown in Fig. 2 for the double barrier heterostructure with an Al concentration of z = 0.50, a barrier width of b = 60 Å, and a well width of a = 50 Å, where we have plotted the ln$T$ *vs* E_x for four different values of k_o . Curves solid, dashed, dotted, and doted-dashed are correspond to different k_o = 0.00, 0.03, 0.05, and 0.07 Å^{-1}, respectively. From the plot in Fig. 2, we find that two sharp peaks shift toward the low-energy region with the increase of the transverse wave number k_o. Moreover, the shift of the second peak is much greater than that of the first peak. In addition, it is also noted that with an increase of k_o the width of resonant peaks broadens, and the peaks reduced with respect to the valley in the transmission spectrum. It is evident that the influence of the transverse motion of the electron on higher resonant states for resonant tunneling is more remarkable than on the lower resonant states.

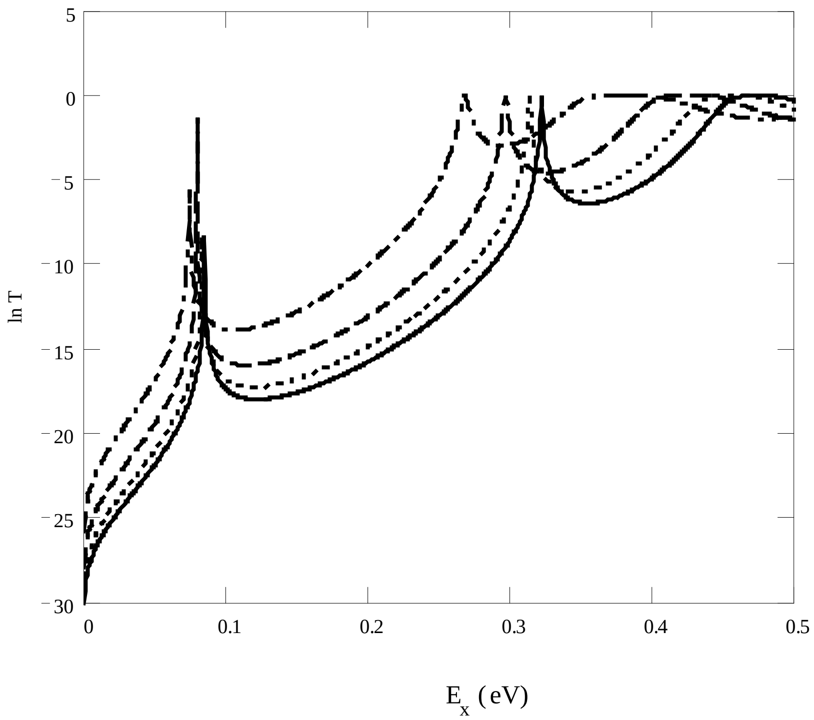

FIG. 2. Natural logarithm of the transmission coefficient *T* as a function of the longitudinal kinetic energy E_x for double barrier heterostructure with parameters: *a* = 50 Å, *b* = 60 Å, and *z* = 0.50. Curves solid, dashed, dotted, and doted-dashed are correspond to the cases of k_o = 0.00, 0.03, 0.05, and 0.07 $Å^{-1}$, respectively.

The results as shown in Fig. 2 can be interpreted from the expression of the effective barrier height in Eq. 4. The increase of the transverse wave number leads to a decrease of the effective barrier height. Consequently, effects such as the shift of resonant peaks, width broadening, and the reduction of peaks are natural consequences of the decrease of the effective barrier height.

Drawing the transmission coefficient *T* as function of the barrier width (*b*) provides some further insight into the influence of transmission coefficient by the coupling effects. This is shown in Fig. 3 for the triple barrier structure with an Al concentration of *z* = 0.3, longitudinal kinetic energy E_x = 400 meV, barrier width is equal to the well width, and for two different values of k_o. Curves solid and dashed correspond to two different values of k_o = 0.00, and 0.05 $Å^{-1}$, respectively. We note that, with the increase of k_o the conduction bands move toward the low-width region and the shifts of the conduction bands at higher widths are much larger than those of the lower ones.

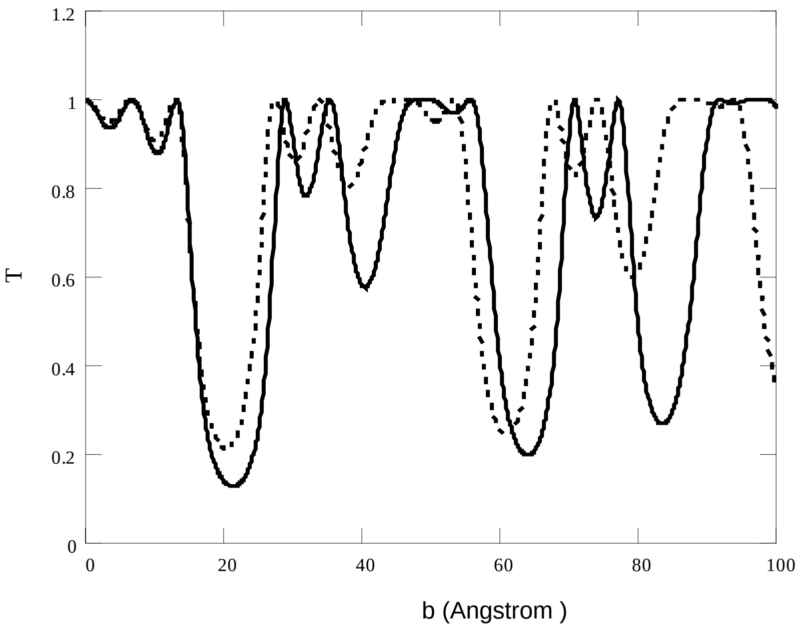

FIG. 3. Transmission coefficient T as a function of the barrier width b for triple barrier heterostructure. The parameters are as follow $a = b$, $E_x = 400$ meV, and $z = 0.50$. Solid, and dashed curves correspond to the cases of k_o = 0.00, and 0.05 $Å^{-1}$, respectively.

To conclude this section, Eqs. (16) and (17) show that the increase of z results in both a lift of U_o and an increase of m_b. From Eq. (4) it can be found that the lift of U_o leads to an increase of the effective barrier height, while the increase of m_b play an opposite role [8], leading to a decrease of the effective barrier height. It follows that, the lift of U_o should weaken the coupling effect, while the increase of m_b should strengthen this coupling effect.

In conclusion, we have shown in this paper that the transmission coefficient is significantly altered by the coupling between components of the motion of the electron in directions parallel and normal to the interfaces. In particular, these effects are larger at higher energies.

4. References

1. R. Tsu and L. Esaki, Appl. Phys. Lett. 22, 562 (1973).
2. Y. Cui *et al*., Nano Lett. 3, 149 (2003).

3. B. S. Doyle *et al*., IEEE Elect.Dev. Lett. 24, 263 (2003).
4. T. B. Boykin, Jan P. A. Van der Waget, and J. S. Harris, Phys. Rev. B 43, 4777 (1991).
5. M. S. Kiledjian, J. N. Schulman, and K. L. Wang, Phys. Rev. B 46, 16012 (1992).
6. M. Y. Azbel, Phys. Rev. B 28, 4106 (1983).
7. M. C. Payen, J. Phys. C 19, 1145 (1986).
8. Xue-Hua Wang *et al*, Phys. Rev. B 55, 9340 (1996).
9. B. Lee, Superlatt. Microstruct. 14, 295 (1993).
10. V. V. Paranjape, Phys. Rev. B 52, 10740 (1995).
11. G. Yong, Y. C. Li, X. J. Kong, and C. W. Wei, Phys. Rev. B50, 17249 (1994).