The Effect of a Position Dependent Effective Mass on the Transmission of Electrons Through a Double Graded Barrier

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Received September 1, 1993; revised manuscript received October 28, 1993

We present a model for the effective mass and barrier potential, to describe the motion of an electron across a nonabrupt double barrier of $GaAs/Al_xGa_{1-x}As/GaAs$. With an interface model, we calculate the transmission coefficient and binding energy of electrons oii a nonabrupt double barrier using tlie multistep potential approximation method. The results obtained show a significant change on the resonant tunneling and energy levels, when compared with those of an abrupt barrier. Numerical results are obtained for different values of the interfacial width and compositional variation of the aluminium.

I. Introduction

The improvement of crystal growth techniques makes possible to produce high-quality layered semiconductor structures such as quantum wells, allowing the observation of man-made quantum size effects in optical devices[1,2]. A particular structure that presents important aplications in several areas is a double barrier heterostructure[3,4]. In this system, the leakage of the electron wavefunction is relevant, allowing the presence of resonant tunneling of electrons through quantum-well states[5]. In order to obtain the physical properties of such systems, one has to solve the Schrödinger equation involving potentials with no-simple profile. Exact analytical solutions of the Schrödinger equation are available only for simple potential structures like the square well. Considering arbitrary potential profile, the Schrödinger equation has been solved numerically, by different methods, such as multistep potential approximation (MPA)[6] and equivalent approach[7,8]. In the MPA method, the variations of potential energy and electron effective mass are approximated by multistep functions, such that continuous variations of potential barriers and effective mass can be analyzed. In this method, the boundary condition has the form that the envelope function, and its derivative divided by effective mass, are continuous at the interfaces. The MPA method has been used to calculate tlie transmission probability through potential barriers[9] and eigenstates in a. quantum well[10].

In most problems involving heterojunctions it is assumed that the interface is abrupt[11,12]. However, experimental results have sliown the absence of atomically smooth semiconductor heterointerfaces[13,14]. Particularly for the case of $GaAs/Al_xGa_{1-x}As$, the transition region of tlie interface can occiir from one to two unit cells[15]. It has been observed that the interfacial width and compositional variation changes considerably the heterostructure properties[16]. Using a nonabrupt potential profile to describe one heterojunction, theoretical calculations have been carried out to analyze tlie transmission coefficient for electrons and holes[17,18].

In this paper, we study the effects of interfacial width and compositional variation on tlic transmission coefficient and binding energy of electrons in a double barrier with interfaces of $GaAs/Al_xGa_{1-x}As$. In Section II we present a. model to describe tlie effective mass, generalized kinetic energy operator and barrier potential. With this model, we calculate tlie transmission coefficient and the binding energy using the MPA approach. In Section III we compare the results obtained as a. function of an interfacial width and compositional

variation of the aluminium.

II. Model description

The system to be studied is a double barrier of $GaAs/Al_xGa_{1-x}As$ with nonabrupt interfaces. Under the effective mass approximation, the envelope function of the electron is given by one-dimensional time-independent Schrödinger equation. We assume that the aluminium molar fraction x changes linearly at the transition regions, Figure 1, and it can be written as

$$\chi(z) = \begin{cases} x(z - z_1)/2a, & z_1 \leq z \leq < z_2, \\ x(z_4 - z)/2c, & z_3 \leq z \leq z_4, \\ x(z - z_5)/2c, & z_5 \leq z \leq z_6, \\ x(z_8 - z)/2a, & z_7 \leq z \leq z_8, \end{cases} \quad (1)$$

where $2b$ is the barrier width; $2a$ and $2c$ are the thickness of the transition regions, d is the distance between the barriers, $z_1 = -d/2 - 2b - a$, $z_2 = z_1 + 2a$, $z_3 = -d/2 - c$, $z_4 = -d/2 + c$, $z_5 = -z_4$, $z_6 = -z_3$, $z_7 = -z_2$, $z_8 = -z_1$ and x is the aluminium molar fraction.

Considering that $Al_xGa_{1-x}As$ conduction band threshold energy dependence on χ is valid for Angstrom dimensions[19], the potential that determines the electron motion in space, shown in Figure 1, is given by

$$V(z) = C(\epsilon_1\chi(z) + \epsilon_2\chi(z)^2) , \quad (2)$$

with C being the band offset, and ϵ_1, ϵ_2 constants associated with the compositional dependence of the energy gap difference between $Al_xGa_{1-x}As$ and GaAs[19].

The electron motion across the barrier is described by a Hamiltonian with a kinetic energy operator, having a position dependent effective mass proposed by von Ross[20],

$$\hat{T} = \frac{1}{4}(m^\alpha \hat{p} m^\beta \hat{p} m^\gamma + m^\gamma \hat{p} m^\beta \hat{p} m^\alpha) , \quad (3)$$

with $\alpha + \gamma + \beta = -1$, $\hat{p}$ as the momentum operator, and m as the effective mass. The effectivc mass in the $Al_xGa_{1-x}As$ is proportional to the aluminium concentration[19]. Considering that this is also true at tlie transition regions, we assume that the effective mass changes continuously according to

$$\frac{m(z)}{m_0} = \mu_1 + \mu_2\chi(z) , \quad (4)$$

where μ_1, μ_2 are parameters obtained experimentally[19], and m_0 is the free electron mass.

In the MPA method we split the potential barrier up into segments. In each one, the potential energy can be regarded as a constant. In tlie limit, a.s the division becomes finer, a continuous variation will be recovered[6].

In our problem we assume that, at the intervals $z_1 < z < z_8$, the potential is divicled in N barriers of width h. At the i^{th} region, the exact solution of the Schrödinger equation for an electron with energy E moving through tlie barrier is given hy

$$\psi_j = A_j e^{ik_{j+1}x} + B_j e^{-ik_{j+1}x} , \quad (5)$$

where

$$k_{j+1} = \sqrt{\frac{2m_{j+1}}{\hbar^2}(E - V_{j+1})} \quad (6)$$

Using generalized boundary conditions[21], the determination of coefficients A_N and B_N is reduccd to matrix equations given by

$$\begin{pmatrix} A_n \\ B_n \end{pmatrix} = \prod_{j=1}^{N} M_j^\beta \begin{pmatrix} A_0 \\ B_0 \end{pmatrix} , \quad (7)$$

where

$$M_j^\beta = \frac{1}{2}\left(\frac{m_{j+1}}{m_j}\right)^{-\alpha} \begin{bmatrix} (1+s_j)e^{-i(k_{j+1}-k_j)x_j} & (1-s_j)e^{-i(k_{j+1}+k_j)x_j} \\ (1-s_j)e^{-i(k_{j+1}+k_j)x_j} & (1+s_j)e^{-i(k_{j+1}-k_j)x_j} \end{bmatrix} , \quad (8)$$

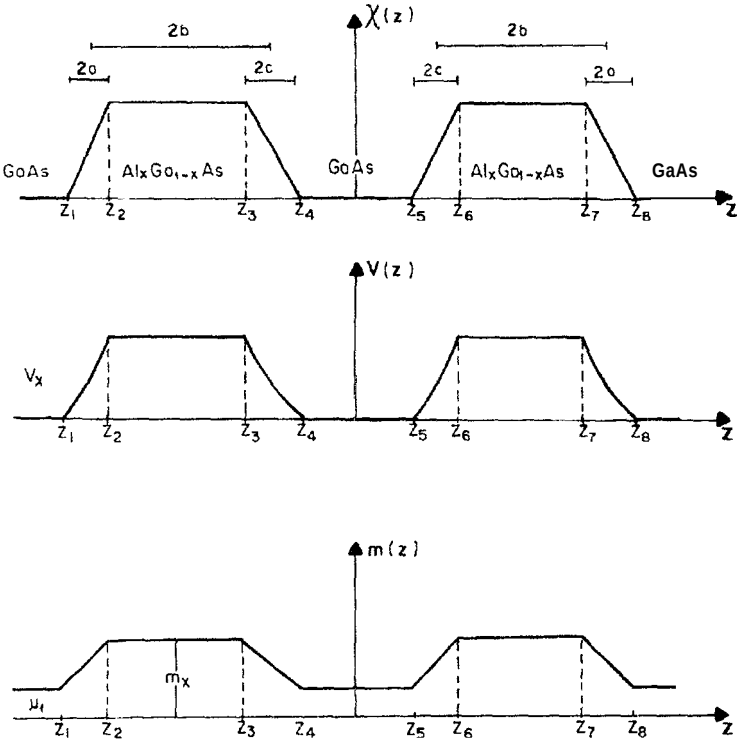

Figure I: Aluminium molar fraction($\Sigma(z)$), potential barrier $V(z)$ and effective mass $m(z)$, as a function of tlie position.

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$$s_j = \frac{k_j}{k_{j+1}} \left(\frac{m_{j+1}}{m_j} \right)^{-\beta} \tag{9}$$

Since in our system tlie effective mass and potential are the same in tlie regions $z < z_1$ and $z > z_8$, and using tlie same procedure of Y. Ando and T. Itoh[6], the transmission coefficient can be written as

$$P_T^\beta = \frac{1}{|M_{22}^\beta|^2} , \tag{10}$$

with

$$M^\beta = \begin{bmatrix} M_{11}^\beta & M_{12}^\beta \\ M_{21}^\beta & M_{22}^\beta \end{bmatrix} = \prod_{j=1}^{n} M_j^\beta . \tag{11}$$

To obtain eigenvalues of an electron on a double barricr we first consider tlie limit $|z_1 - z_8| \to \infty$. Using this fact, the wavefunction, Eq. (5), in the regions $z < z_2$ and $z > z_6$ decay exponentially and as a consequence $B_N = A_0 = 0$, in Eq.(7). With this, eigenvalues are obtained by taking the matrix element M_{22}^β, Eq. (11), as equal to zero.

To compare all results we assume for the kinetic operator, Eq. (3), $\alpha = \gamma = 0$ and $\beta = -1$. Using this, boundary conditions have the form that tlie envelope function of the electron, and its derivative divided by effective mass, are continuous at the interfaces.

III. Results and discussion

In order to obtain numerical results, we use the experimental parameters given in Ref. 19 and consider a conduction band offset of 60%.

To analyse the effects of transition regions we initially consider changes on the externa1 side of the double barrier. In Figure 2 we show the transmission coefficient of electrons, with energies higher than the potential barrier, on an abrupt and nonabrupt double barrier with $d = 100\AA$, $2b = 100\AA$, aluminium molar concentration $x = 0.45$ and a symmetric transition region of widths $2c = 2.0LP$ and $2a = 2.0, 4.0, 6.0LP$, where LP is the lattice parameter of GaAs. When the aluminium concentration decreases, the difference on effective mass is less significant. Consequently, we observe that the difference between results obtained for abrupt and nonabrupt barriers becomes smaller. In Figure 3, we show tlie effects on the transmission coefficient of electrons due to changes on internal transition regions.

Again, me note considerable change ou the transmission coefficient. As observed for a single barrier[17], transition regiors on double barrier produce a. significative effect oii tlie peak-to-valley ratio.

Considering electrons with energies lower than barriers, in Figure 4a we plot the transmission coefficient on a nonabrupt double barrier with $d = 10\AA$, $2b = 200\AA$, aluminium molar concentration $x = 0.45$ aiid a. symmetric transition region of widths $2a = 2.0LP$ and internal transition regions of $2c = 2.0, 4.0, 6.0LP$. As can be seen, transition regions shift tlie peaks of resonant tunneling to higher values of energy. This effect is more significant for peaks of lower energy. This fact is also observed in Figure 4b, where we compare transmission coefficient on a.double barrier with abrupt and nonabrupt interfaces witli $d = 50\AA$, $2b = 100\AA$, aluminium molar concentration $x = 0.45$ and symmetric transition regions of widths $2a = 2.0LP$ and $2c = 6.0LP$. Again, the effect of the transition region is more significative for lower peak of resonant tunneling. We observed that for energies lower than the barrier potential, the transition regions external to double barrier do not have a significant effect on resonant tunneling.

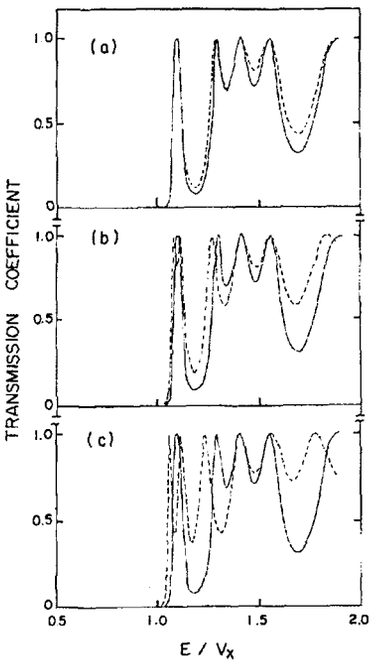

Figure 3: Transrnission coefficient as a function of incident electron energy, on a double barrier with d = $100\AA$, $2b = 100\AA$, aluminium molar concentration $x = 0.45$ and symmetric transition regions of widths $2a = 2.0LP$, considering abrupt barriers (—) and $2c = 2.0LP$ (a), $2c = 4.0LP$ (b), $2c = 6.0LP$ (c).

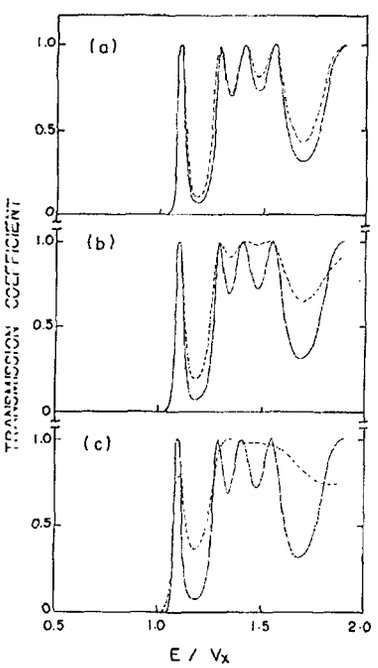

Figure 2: Transmission coefficient as a function of incident electron energy, on a double barrier with $d = 100\AA$, $2b = 100\AA$, aluminium molar concentration $x = 0.45$ and symmetric transition regions of widths $2c = 2.0LP$, considering abrupt barriers (—) and $2a = 2.0LP$ (a): $2a = 4.0LP$ (b). $2n = 6.0LP$ (c).

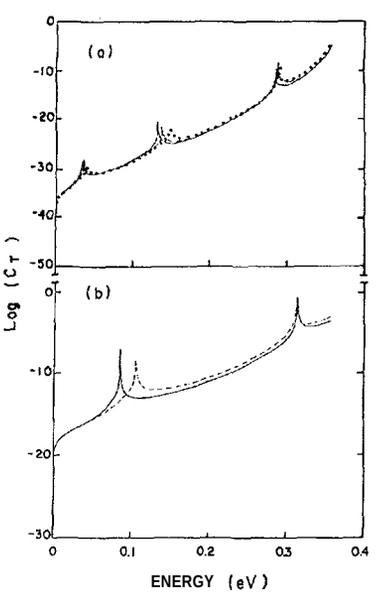

Figure 4: 'Transrnission coefficient as a fnnction of incident electron energy, on a double barrier with aluminiiim molar concentration x = 0.45: considering: (a) nonabrupt barriers with synimetric transition regions with d = $100\AA$, $2b = 200\AA$, $2a = 2.0LP$, $2c = 2.0LP$ (—) $2c = 4.0LP$ (- - -) and $2c = 6.0LP$ (....); (b) abrupt (—-) and nonabrupt barrier (- - -) with $d = 50\AA$, $2b = 100\AA$, $2a = 2.0LP$ and $2c = 6.0LP$.

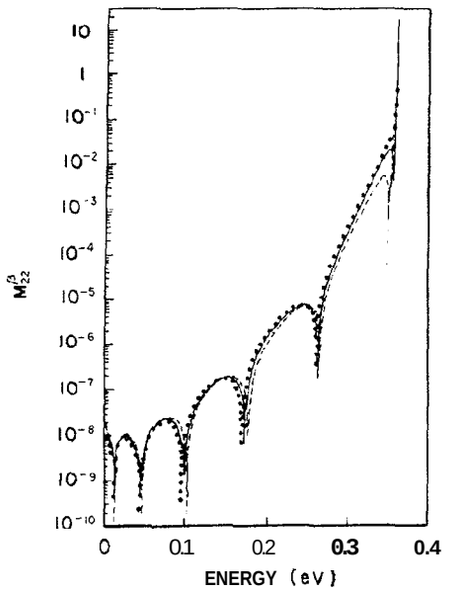

Figure 5: Matrix element M_{22}^3 as a function of electron energy for an aluminium molar concentration $x = 0.43$. nonabrupt barriers with symmetric transition regions with $d = 200\AA$, $2c = 2.0LP$ (...), $2c = 4.0LP$ (--). and $2c = 6.0LP$ (- - -).

Since the eigenvalues of an electron in a double barrier are obtained by searching foi zeros of M_{22}^3, in Fig. 5 we plot it as a function of electron energy considering $d = 200\AA$, aluminium molar concentration $x = 0.15$ and symmetric transition regions of widths $2c = 2.0, 4.0$ and $6.0LP$. The resonances correspond to eigenvalues energies. These results are consistent with those obtained in the resonant tunneling, since the transition regions shift the eigenvalues to higher energies.

In conclusion, the effect of a transition region on tlie transmission coefficient and eigenvalues energies of an electron in a double barrier heterostructure is significant. Since in these systems we consider an effective mass which changes continuously through the transition regions, we cxpect that our model represents a more realistic picture of nonabrupt double barrier systems.

Acknowledgments

This work was supported in part by CNPq and FINEP.

References

1. R. M. líolbas and N. Holonyak Jr., Am. J. Phys. 52, 431 (1984).
2. K. Hess and N. Holonyak Jr., Pliys. Today **33,** 40 (1980).
3. D. Roy, *Quantum Mechanical Tunneling* ***and its*** *Application* (World Scientific, Singapore, 1986).
4. G. Kin and G. B. Arnold, Pliys. Rev. B**38**, 3252 (1088).
5. L. Chang, L. Esaki and R. Tsu, Appl. Phys. Lett. **24**, 593 (1974).
6. Y. Ando and T. Itoh, J. Appl. Phys. 61, 1497 (1987).
7. R. Wait and A. R. Mitchell, *Finite Element Analysis and Applications*, (Wiley, London, 1966) p.1.
8. W. W. Lui and M. Fukuma, J. Appl. Phys. 60, 1555 (1986).
9. K. Nakamura, A. Shimizu and M. Koshiba, IEEE J. Quantum Electron. QE-**27**, 1189 (1991).
10. K. Nakamura, A. Shimizu and M. Koshiba, IEEE J. Quantum Electron. QE-25, 889 (1989).
11. L. A. K. Cury and N. Studart, Superlatt. Microstruc. **3,** 175 (1987).
12. L. Esaki, IEEE J. Quantum Electron. QE-22, 1611 (1986).
13. M. Zachau and D. Guitzmacher,' Appl. Phys. Lett. 56, 692 (1090).
14. C. A. Warwick, W. Y. Jan and A. Gurmazd, Appl. Phys. Lett. 56, 2666 (1990).
15. O. Albrektsen, D. J. Aren, H. P. Meier and H. W. M. Salemick, Appl. Pliys. Lett. 57, 31 (1990).
16. J. S. Schulman, Appl. Phys. Lett. 44, 644 (1983).
17. V. N. Freire, G. A. Farias and M. M. Auto, Superlatt. Microstruc. **11**, 17 (1992).
18. V. N. Freire, G. A. Farias and M. M. Auto, J. Appl. Phys. **71**, 4076 (1992).
19. S. Adachi, J. Appl. Pliys. 58, R1 (1985).
20. G. von Ross, Phys. Rev. B**27**, 7547 (1983).
21. R. *h.* Monow and K. R. Brownstein, Phys. Rev. B**30**, 678 (1984).