Electron Transmission Through Nonabrupt $GaAs/Al_xGa_{1-x}As$ Double-Barriers Subjected to an Electric Field

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It is shown that the existence of nonabrupt interfaces modify electric field effects on the electron transmission through a $GaAs/Al_xGa_{1-x}As$ double-barrier. When the applied electric intensity is $25\,kV/cm$, and the abrupt well and barriers are $100\,Å$ wide, interfaces as thin as two GaAs lattice parameters are responsible for shifts at least of $10\,meV$ in the electron tunneling resonance energies. The type of interface potential and electron effective mass description changes significantly theoretical results related to the electric field influence on the electron transmission properties.

I. Introduction

It is a great pleasure for us to contribute with this paper to the special number of the Brazilian Journal of Physics in honor to Prof. Dr. Roberto Luzzi on the special occasion of his sixtieth anniversary. One of the authors, V. N. Freire, had the opportunity to be formally one of his PhD students at the Universidade Estadual de Campinas (UNICAMP), in Campinas, Brasil.

Although considerably attention has been given to the study of carrier tunneling phenomena through double-barrier semiconductor heterostructures (DBSH),[1-4] only recently it was shown that interface effects are important to be take into account for an improved description of their tunneling characteristics. In the sequential tunneling picture, interfaces are considered as an important mechanism to obtain smaller peak-to-valley ratios in the tunneling current.[5-7] The influence of interface roughness on coherent tunneling of single and double-barriers was also shown to be relevant.[8-10] However, in both the sequential and coherent tunneling picture, interface effects are generally investigated within the assumption of the existence of islands at an otherwise abrupt semiconductor interface.[5-10]

Graded interface effects, *i.e.*, smooth interfacial variations of the semiconductor alloy are also important in the coherent tunneling picture of single[11] and double barriers.[12] In this case, interface widths as small as two lattice parameters (LP) can change considerably the tunneling behavior of carriers through semiconductor barriers. Since experiments have estimated that $GaAs/Al_xGa_{1-x}As$ interfacial regions have widths of the order of two lattice parameters,[13-14] it was suggested that some disagreement between theory and experiment in DBSH tunneling may be related with nonabrupt interface characteristics.[12] In fact, the interfaces of the quantum well in a $GaAs/Al_xGa_{1-x}As$ DBSH determine the energy of the transmission resonance peaks and an increase of the interfacial widths of the quantum well shifts the transmission resonances.[12]

Since the existence of nonabrupt interfaces reduces (enhances) the Stark shift of the electron ground state energy (first excited electron energy level) in a single nonabrupt $GaAs/Al_xGa_{1-x}As$ quantum well,[15] interface effects modify the transmission properties of

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carriers through DBSH subjected to an electric field. The electron transmission through a single nonabrupt GaAs/Al$_x$Ga$_{1-x}$As barrier subjected to an electric field was shown to depend strongly on the interface potential and carrier effective-mass description.(16) In this case, the electron transmission is reduced both by the electric field induced asymmetry and the existence of nonabrupt interfaces.(16)

The purpose of this paper is to investigate the influence of nonabrupt interfaces in the transmission properties of an electron through a GaAs/Al$_x$Ga$_{1-x}$As double-barrier subjected to an electric field. The GaAs/Al$_x$Ga$_{1-x}$As nonabrupt interface model is described in the Section II, the results of the transmission calculations of electrons through nonabrupt GaAs/Al$_x$Ga$_{1-x}$As double-barriers are discussed in the Section III. The Section IV closes this work with the presentation of the main conclusions.

II. The nonabrupt GaAs/Al$_x$Ga$_{1-x}$As double-barrier model

The GaAs/Al$_x$Ga$_{1-x}$As interfaces are described according the Al$_{\mathcal{X}(z)}$Ga$_{1-\mathcal{X}(z)}$As alloy variation in the interface regions. The double-barrier growth is in the z direction and $\mathcal{X}(z)$ is a function that describes the aluminum molar fraction variation in the interfacial regions. Actually, the interfacial alloy variation profile depends on the conditions and growth techniques of the semiconductor sample. Interfacial growth patterns influence the properties of semiconductor heterostructures, as can be infered from the role of growth interface interruptions on the luminescense properties of semiconductor quantum wells.(17) Transmission properties of carriers through nonabrupt GaAs/Al$_x$Ga$_{1-x}$As single barriers were shown to depend on the interfacial growth pattern of the aluminum molar fraction.(18) However, a linear variation for $\mathcal{X}(z)$ is assumed here because: (i) it allows to obtain analytical expressions for the transmission coefficient in the constant interfacial effective-mass approximation; (ii) it is the simplest nontrivial approximation for any kind of semiconductor alloy variation.

With the method first proposed by Freire, Auto, and Farias,(19) the inter-related interface potential and electron effective mass are obtained from $\mathcal{X}(z)$. In this case, the electron effective mass is position dependent, $m = m(z)$, and a kinetic energy operator with position dependent effective mass has to be employed. Several forms for the kinetic energy operator were proposed,(20) and while controversy exist about the best choice,(20–26) the most used is that proposed originally by BenDaniel and Duke,(27) $(-\hbar^2/2)(d/dz)[m(z)]^{-1}(d/dz)$. With this operator, the quantum behavior of an electron tunneling through a nonabrupt GaAs/Al$_x$Ga$_{1-x}$A double-barrier subjected to an electric field (see Fig. 1), is described by the following Schrödinger-like equations:

• $z \leq z_1$

$$-\frac{\hbar^2}{2M_{MIN}}\frac{d^2\Psi(z)}{dz^2} = E\Psi(z)\ ; \tag{1}$$

• $z_1 \leq z \leq z_2$

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left\{\left[\mathcal{M}_{2,1}(z)\right]^{-1}\frac{d\Psi(z)}{dz}\right\}+ \left[\mathcal{V}_{2,1}(z)+V_F(z)\right]\Psi(z) = E\Psi(z)\ ; \tag{2}$$

• $z_2 \leq z \leq z_3$

$$-\frac{\hbar^2}{2M_{MAX}}\frac{d^2\Psi(z)}{dz^2} + \left[V_{MAX}+ V_F(z)\right]\Psi(z) = E\Psi(z)\ ; \tag{3}$$

• $z_3 \leq z \leq z_4$

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left\{\left[\mathcal{M}_{3,4}(z)\right]^{-1}\frac{d\Psi(z)}{dz}\right\}+ \left[\mathcal{V}_{3,4}(z)+V_F(z)\right]\Psi(z) = E\Psi(z)\ ; \tag{4}$$

• $z_4 \leq z \leq z_5$

$$-\frac{\hbar^2}{2M_{MIN}}\frac{d^2\Psi(z)}{dz^2} + V_F(z)\Psi(z) = E\psi(z)\ ; \tag{5}$$

• $z_5 \leq z \leq z_6$

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left\{\left[\mathcal{M}_{6,5}(z)\right]^{-1}\frac{d\Psi(z)}{dz}\right\}+ \left[\mathcal{V}_{6,5}(z)+V_F(z)\right]\Psi(z) = E\Psi(z)\ ; \tag{6}$$

• $z_6 \le z \le z_7$

$$-\frac{\hbar^2}{2M_{MAX}}\frac{d^2\Psi(z)}{dz^2}+$$
$$\left[V_{MAX}+V_F(z)\right]\Psi(z)=E\Psi(z)\ ; \quad (7)$$

• $z_7 \le z \le z_8$

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left\{\left[\mathcal{M}_{7,8}(z)\right]^{-1}\frac{d\Psi(z)}{dz}\right\}+$$
$$\left[\mathcal{V}_{7,8}(z)+V_F(z)\right]\Psi(z)=E\Psi(z)\ ; \quad (8)$$

• $z \ge z_8$

$$-\frac{\hbar^2}{2M_{MIN}}\frac{d^2\Psi(z)}{dz^2}=\left[E-V_F(z_8)\right]\Psi(z)\ . \quad (9)$$

In the preceding equations,

$$\mathcal{V}_{i,j}(z)=Q_e\left[V_0(z_i,z_j)+V_1(z_i,z_j)z+\right.$$
$$\left.V_2(z_i,z_j)z^2\right]\ ; \quad (10)$$

$$\mathcal{M}_{i,j}(z)=m^*\left[m_0(z_i,z_j)+m_1(z_i,z_j)z\right]\ ; \quad (11)$$

$$V_F(z)=qE_F(z-z_1)\ ; \quad (12)$$

$$V_0(z_i,z_j)=-\varepsilon_1\left(\frac{x}{z_i-z_j}\right)+\varepsilon_2{z_1}^2\left(\frac{x}{z_i-z_j}\right)^2\ ; \quad (13)$$

$$V_1(z_i,z_j)=-\varepsilon_1\left(\frac{x}{z_i-z_j}\right)-2\varepsilon_2\left(\frac{x}{z_i-z_j}\right)^2\ ; \quad (14)$$

$$V_2(z_i,z_j)=\varepsilon_2\left(\frac{x}{z_i-z_j}\right)^2\ ; \quad (15)$$

$$m_0(z_i,z_j)=\mu_1-\mu_2 z_1\left(\frac{x}{z_i-z_j}\right)^2\ ; \quad (16)$$

$$m_1(z_i,z_j)=\mu_2\left(\frac{x}{z_i-z_j}\right)^2\ ; \quad (17)$$

$$V_{MAX}=Q_e\left[\varepsilon_1+\varepsilon_2 x^2\right]\ ; \quad (18)$$

$$M_{MAX}=m^*\left[\mu_1+\mu_2 x\right]\ ; \quad (19)$$

$$M_{MIN}=m^*\mu_1\ , \quad (20)$$

where E is the electron energy, z_i the interfaces coordinates, x the $Al_xGa_{1-x}As$ aluminum molar fraction, q the electron charge, E_F the intensity of the applied electric field, Q_e the electron band offset, and m^* the free-electron mass. The parameters ε_i (μ_i) are obtained from experiments, and are related with the compositional dependence of the $Al_xGa_{1-x}As$ electron effective mass (energy gap) in the Γ direction.[19] According to Adachi,[28] $\varepsilon_1 = 1.155$, $\varepsilon_2 = 0.37$, $\mu_1 = 0.067$, and $\mu_2 = 0.083$.

The ensemble of equations (1-9) can be solved analitically by disregarding the linear spatial dependence of the interfacial electron effective mass - the so called constant interfacial effective-mass (CIEM) approximation,[19,29] and by imposing matching conditions on $\Psi(z)$ and $[m(z)]^{-1}d\Psi(z)/dz$ at z_i, $i=1,\ldots,8$ (see Fig. (1)). Beyond the CIEM approximation, only a numerical solution of the Eqs. (1-9) is possible. In this case, the numerical method of Ando and Itoh[30] was used to solve the equations.

III. Numerical Results and Discussion

The electron transmission coefficient T_{pl} is calculated considering the parabolic interface potential and the linear dependence of the interfacial electron effective mass. In the CIEM approximation, both the linear and the constant potential approximations are used to obtain the transmission coefficients T_{lc} and T_{cc}, respectively. A comparison between these coefficients and the transmission coefficient T_{ab}, calculated in the abrupt interface picture, shows the significance of the inclusion and a good modelling of interfaces to the description of electron transmission properties through $GaAs/Al_xGa_{1-x}As$ double-barrier subjected to an electric field.

Figure 1 depicts the potential and electron effective mass associated to $GaAs/Al_xGa_{1-x}As$ double-barriers subjected to an electric field. Both the abrupt well and barriers are 100 Å wide. The AlGaAs aluminum molar fraction content is $x = 0.35$, the maximum height of the first barrier is $V_{MAX} = 270\,meV$, the electron band offset is $Q_e = 0.6$, and R_G (R_A) are GaAs ($Al_{0.35}Ga_{0.65}As$) regions. According experimental results,[13,17,31,32] interfacial regions of $Al_xGa_{1-x}As$ grown in GaAs (R_{GA} regions) have a roughness degree stronger than interfacial regions of GaAs grown in $Al_xGa_{1-x}As$ (R_{AG} regions). While this interfacial asymmetry is impossible to be take into account within the abrupt interface picture, it is described here by considering simply that R_{GA} regions are wider than R_{AG} regions. The interface widths are: $2\,LP$ for R_{GA} regions and $1\,LP$ for R_{AG} regions in Figs. 2 and 3; $4\,LP$ for R_{GA} regions and $1\,LP$ for R_{AG} regions in Figs. 4 and 5. For all the interfaces, the applied electric field intensities are $E_F = 0$, 25, 55, and $85\,kV/cm$.

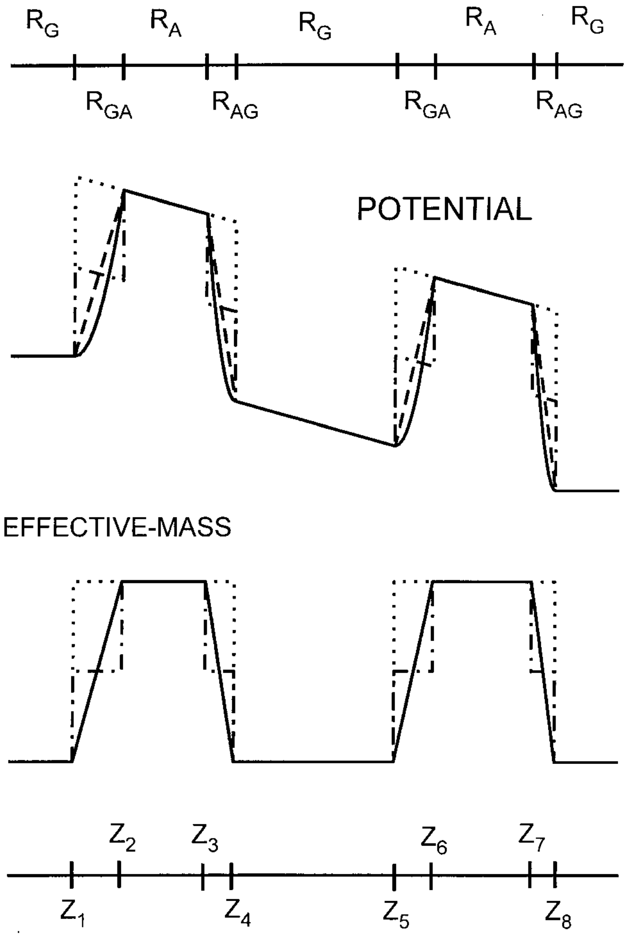

Figure 1. $GaAs/Al_xGa_{1-x}As$ double-barrier potential and electron effective mass. In the case of the potential: the abrupt potential picture (dotted); the parabolic potential variation (solid); the linear potential variation (dashed); the constant potential approximation (dotted dashed) - inclined in the figure by the action of the electric field E_F. In the case of the electron effective mass: the abrupt effective-mass picture (dotted); the linear effective-mass variation (solid); the constant effective-mass approximation (dotted dashed).

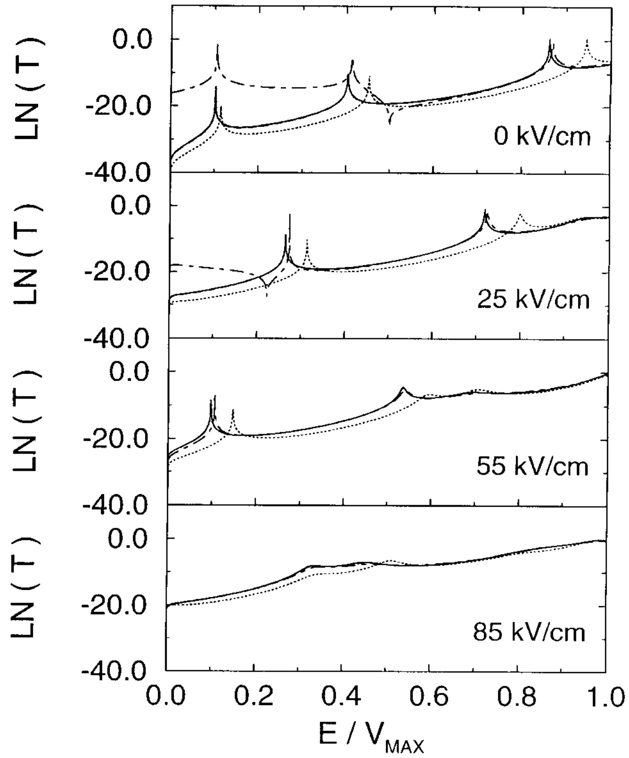

Figure 2. Transmission coefficients of electrons through single $GaAs/Al_{0.35}Ga_{0.65}As$ double-barriers subjected to electric field intensities of $0\,kV/cm$, $25\,kV/cm$, $55\,kV/cm$, and $85\,kV/cm$, considering: abrupt interfaces, T_{ab} (short dashed); the parabolic potential and the linear electron effective mass in the interfacial regions, T_{pl} (solid); the linear potential and the constant electron effective mass approximation in the interfacial regions, T_{cc} (long dashed) - it is always almost identical to T_{pl} in the figure; the constant potential and the electron effective mass approximation in the interfacial regions, T_{lc} (dotted dashed). A band offset $Q_e = 0.6$, an aluminium molar fraction $x = 0.35$, and interface widths of $2\,LP$ were used. The abrupt barriers and well widths were of 100 Å, and the electron energy was $0 < E < V_{MAX}$.

When $E < V_{MAX}$, one could see in Fig. 2 that not only the number of tunneling resonances can be reduced for suficiently high electric fields, but that this number depends also on the widths of the nonabrupt double-barrier interfaces. Three tunneling resonances occur in the absence of an electric field, two exist when $E_F = 25\,kV/cm$, and none is present in the case of high electric fiels, $E_F \gtrsim 85\,kV/cm$. Electron tunneling resonance energies are always smaller in the case of nonabrupt interfaces. High order resonances are more influentiated by the existence of nonabrupt interfaces than low order resonances. When $E_F = 25\,kV/cm$, the first (second) tunneling resonance energy of T_{pl} are shifted toward low energies in comparison to that of T_{ab}

by as much as $13\,meV$ ($22\,meV$). By comparing T_{ab}, T_{pl}, T_{lc}, and T_{cc}, it is observed that always $T_{lc} \simeq T_{pl}$. On the other hand, the constant interface potential and electron effective-mass approximation is good for interface modelling when $E_F \gtrsim 55\,kV/cm$ and $E < V_{MAX}$, since in this case $T_{pl} \simeq T_{cc}$. If $E_F \gtrsim 85\,kV/cm$, the differences between abrupt and nonabrupt interfaces are unimportant.

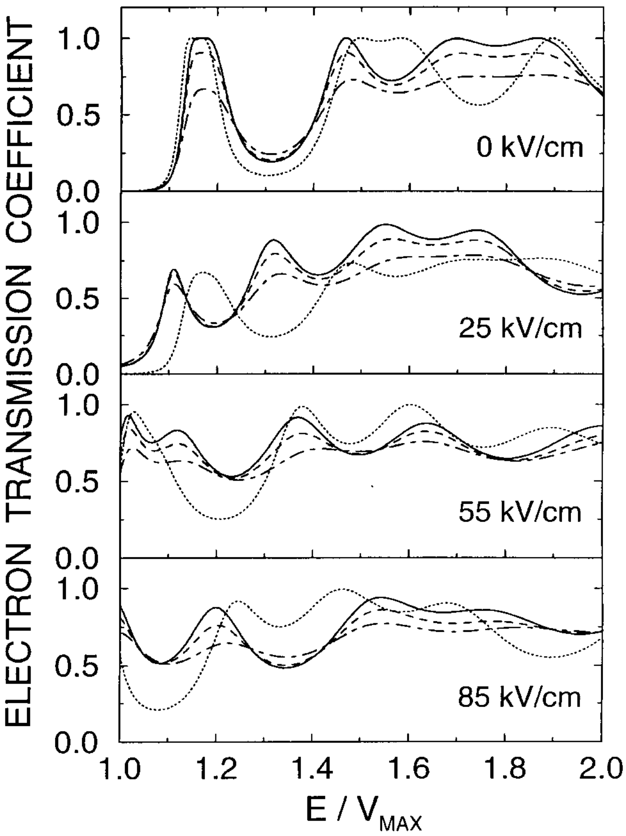

Figure 3. Transmission coefficients of electrons through single GaAs/$Al_{0.35}Ga_{0.65}As$ double-barriers subjected to electric field intensities of $0\,kV/cm$, $25\,kV/cm$, $55\,kV/cm$, and $85\,kV/cm$, considering: abrupt interfaces, T_{ab} (short dashed); the parabolic potential and the linear electron effective mass in the interfacial regions, T_{pl} (solid); the linear potential and the constant electron effective mass approximation in the interfacial regions, T_{cc} (long dashed) - it looks like T_{pl} in the low energy region of the figure; the constant potential and the electron effective mass approximation in the interfacial regions, T_{lc} (dotted dashed). A band offset $Q_e = 0.6$, an aluminium molar fraction $x = 0.35$, and interface widths of $2\,LP$ were used. The abrupt barriers and well widths were of 100 Å, and the electron energy was $V_{MAX} < E < 2$.

When $E > V_{MAX}$, the role of interfaces on the transmission properties of electrons through nonabrupt $Al_{0.35}Ga_{0.65}As$ double-barriers are important even when $E_F = 85\,kV/cm$ (see Fig. 3). If no electric field is applied, the first transmission peak of T_{ab}, T_{pl}, T_{lc}, and T_{cc} are very similar, and occur approximately at the same electron energy. When an electric field is applied, the positions of the transmission peaks of T_{pl}, T_{lc}, and T_{cc} are very close, but are shifted toward low energies in comparison with that of T_{ab}. The CIEM approximation smooths the transmission peaks, and in general $T_{pl} > T_{lc} > T_{cc}$.

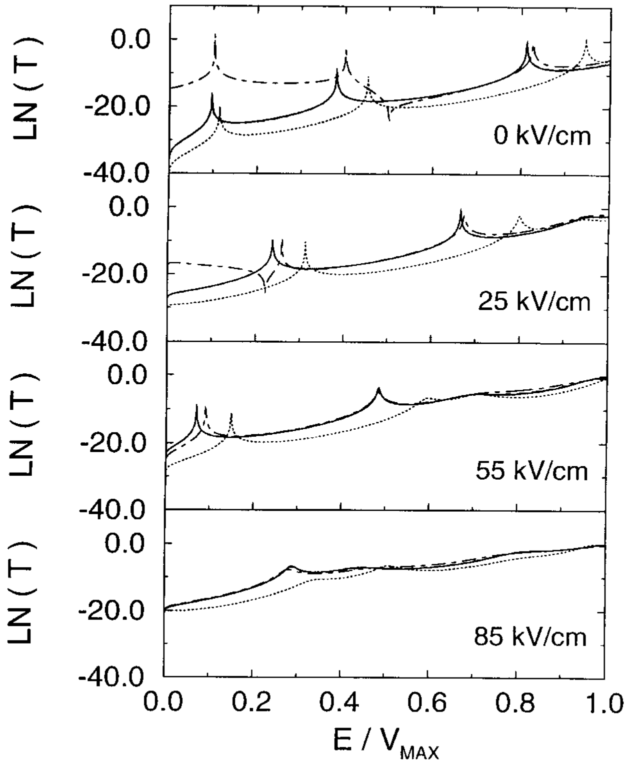

Figure 4. Transmission coefficients of electrons through single GaAs/$Al_{0.35}Ga_{0.65}As$ double-barriers subjected to electric field intensities of $0\,kV/cm$, $25\,kV/cm$, $55\,kV/cm$, and $85\,kV/cm$, considering: abrupt interfaces, T_{ab} (short dashed); the parabolic potential and the linear electron effective mass in the interfacial regions, T_{pl} (solid); the linear potential and the constant electron effective mass approximation in the interfacial regions, T_{cc} (long dashed) - it is always almost identical to T_{pl} in the figure; the constant potential and the electron effective mass approximation in the interfacial regions, T_{lc} (dotted dashed). A band offset $Q_e = 0.6$, an aluminium molar fraction $x = 0.35$, and interface widths of $4\,LP$ were used. The abrupt barriers and well widths were of 100 Å, and the electron energy was $0 < E < V_{MAX}$.

When the widths of the R_{GA} regions increase, the transmission phenomena related with interfaces are enhanced. By comparing Figs. 4 and 5 (obtained with R_{GA} interfaces of $4\,LP$) with Figs. 2 and 3 (obtained with R_{GA} interfaces of $2\,LP$), one verify that the differences between the tunneling resonance energies of T_{ab} and T_{pl} have increased. In Fig. 4, the first (second) tunneling resonances of T_{ab} and T_{pl} have a difference of 20 meV (37 meV) when $E_F = 25\,kV/cm$. When $E > V_{MAX}$ (see Fig. (5)), the differences between the transmission ($E > V_{MAX}$) coefficients T_{pl}, T_{lc}, and T_{cc} increase. All of them are more smooth. Finally, the reduction of T_{pl}, T_{lc}, and T_{cc} with the intensity of the electric field is smaller when the interfaces are wider.

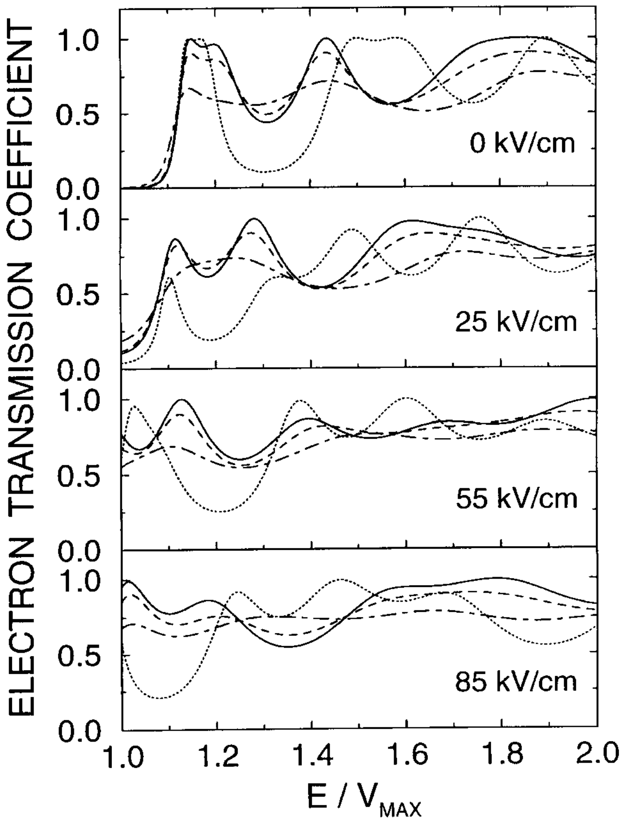

Figure 5. Transmission coefficients of electrons through single $GaAs/Al_{0.35}Ga_{0.65}As$ double-barriers subjected to electric field intensities of $0\,kV/cm$, $25\,kV/cm$, $55\,kV/cm$, and $85\,kV/cm$, considering: abrupt interfaces, T_{ab} (short dashed); the parabolic potential and the linear electron effective mass in the interfacial regions, T_{pl} (solid); the linear potential and the constant electron effective mass approximation in the interfacial regions, T_{cc} (long dashed) - it looks like T_{pl} in the low energy region of the figure; the constant potential and the electron effective mass approximation in the interfacial regions, T_{lc} (dotted dashed). A band offset $Q_e = 0.6$, an aluminium molar fraction $x = 0.35$, and interface widths of $4\,LP$ were used. The abrupt barriers and well widths were of 100 Å, and the electron energy was $V_{MAX} < E < 2$.

Our results indicate that the existence of $GaAs/Al_xGa_{1-x}As$ interfaces as thick as $2\,LP$ in double-barriers samples could be responsible for considerable disagreement between experiments and theoretical results obtained in the abrupt interface picture. Since the best grown $GaAs/Al_xGa_{1-x}As$ samples have nowadays interface widths of the order of $2\,LP$,[13,14] it seems always necessary to consider the existence of nonabrupt interfaces for a better description of $GaAs/Al_xGa_{1-x}As$ double-barrier properties.

IV. Concluding remarks

Experiments on electron tunneling through semiconductor barriers are very scarce. The technique used by Choi, Newman, and Iafrate,[33] carefully designed to observe coherent tunneling, may be used to probe the influence of interfaces on the electron energy tunneling resonances of $GaAs/Al_xGa_{1-x}As$ double-barrier heterostructures. On the other hand, the measurements of the reflection and transmission coefficients of ballistic two-dimensional electrons by Ying *et al.*[34] indicate that they are very sensitive to the barrier shape, principally nonabrupt interfaces. However, experimental evidences of interface effects on the electron transmission through $GaAs/Al_xGa_{1-x}As$ double-barriers subjected to an electric field were not obtained up to now. The transmission calculations performed here are now being used by the present authors in the calculation of current $\times$ voltage curves of $GaAs/Al_xGa_{1-x}As$ double-barrier heterostructures to be compared with experimental measurements.

Since the main interest in this work is the study of the role of interfaces on the transmission properties of undoped $GaAs/Al_xGa_{1-x}As$ double-barrier heterostructures, the calculations were performed without considering charge accumulation in the emitter and well regions. On the other hand, accumulation layer and interface effects must be take into account when high doped nonabrupt $GaAs/Al_xGa_{1-x}As$ heterostructures are studied. Recently, Freire *et al*[35] showed that interfacial effects on the electron energy levels of doped nonabrupt $GaAs/Al_xGa_{1-x}As$ heterojunctions are more (less) important for high doping levels (small band bending widths). They have calculated energy level corrections associated to the existence of band bending and interface effects that are almost one order higher than those obtained by Stern and Das Sarma[36] in the case of wide accumulation layers and small tickness of the $GaAs/Al_xGa_{1-x}As$ interfaces.

To conclude, it was shown that interface effects have to be considered for a better description of the electron transmission through $GaAs/Al_xGa_{1-x}As$ double-barriers subjected to an alectric field. Errors at least of the order of 10 meV in the tunneling resonances energies may be frequent when comparison between experimental results obtained with actual semiconductor samples and theoretical calculations based in the abrupt interface picture are done.

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