Electron transmission through a single nonabrupt GaAs/Al_xGa_{1-x}As barrier subjected to an electric field

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Calculations of the electron transmission through a single nonabrupt GaAs/Al_xGa_{1-x}As barrier subjected to an electric field have been performed. The electron transmission is shown to be strongly dependent on the interface potential and electron effective mass. The overall reduction of the electron transmission due to the electric field is smaller for wide interfaces. Peak-to-valley transmission ratios change considerably with the interfacial width, as well as with the scheme used to describe interfaces.

Since the original work of Tsu and Esaki,[1] much effort has been devoted to fundamental and applied research on transmission properties of semiconductor multibarrier heterostructures. Although device applications like resonant tunneling diodes and transistors, photoconductors, photodetectors, and light emitters have been implemented,[2] some important difficulties related to the subject are not completely resolved up to now. Coherent versus sequential-tunneling descriptions and theoretical overestimation of peak-to-valley current (PVC) ratio measurements are among the unsolved problems of low-dimensional semiconductor physics.

In the sequential-tunneling picture, carrier-scattering mechanisms with carriers, phonons, impurities, and rough interfaces reduce the PVC ratio,[3] but they do not explain the overestimation definitively. In the coherent-tunneling picture, corrections of the Tsu-Esaki formula,[4] and effects of spatially variable effective mass[5] and interface roughness,[6] are considered as mechanisms reducing PVC ratios. In both pictures, interface effects are introduced in a restrictive way, as a consequence of the limitations of the models proposed to describe the interfaces. Roughness associated with abrupt interface islands of variable surface and height,[6] as well as graduated heterojunction interfaces,[7] are shown to be important elements to be considered if a better interface representation is sought.

The variable interfacial alloy composition modifies both the potential and the carrier effective mass in an inter-related manner. It was shown recently that carrier transmission through a nonabrupt GaAs/Al_xGa_{1-x}As heterojunction depends on the interfacial type of aluminum molar fraction variation $\mathcal{X}(z)$.[8] When $\mathcal{X}(z)$ is a linear function, with values 0 and x at the limits $-a$ and $+a$ of the interface, respectively, the potential in this region is a quadratic function of the coordinate z in the growth direction, while the carrier effective mass is a linear function. With this description of the interface region, Renan *et al.*[7] showed that the transmission coefficient of a nonabrupt GaAs/Al_xGa_{1-x}As single barrier has significant differences from that obtained with an abrupt barrier, even when the interfacial widths are of two lattice parameters GaAs (2 LP), i.e., of the order of the smallest interfacial width obtained with present heterojunction growth techniques.[9,10] By using the same interfacial model, Ribeiro Filho, Farias, and Freire[11] have presented calculations of the transmission properties of nonabrupt GaAs/Al_xGa_{1-x}As heterojunctions, and indicated that the frequently used assumption of a linear potential and a constant effective mass in the interface region should be regarded with caution.

In this work, we study the role of interfaces in the transmission properties of an electron through a GaAs/Al_xGa_{1-x}As single barrier subjected to an electric field. To describe the effects of nonabrupt interfaces of the GaAs/Al_xGa_{1-x}As single barriers subjected to an electric field, we use the assumption of the linear dependence of $\mathcal{X}(z)$ through the interfaces. The interface potential and the electron effective mass, depicted in Figs. 1(a) and 1(b), respectively, are obtained following the method first proposed by Freire, Auto, and Farias.[12] Analytical expressions for them are presented in Table I, where

$$V_{0,r}=Q_e[\varepsilon_1 b(x/r)+\varepsilon_2 b^2(x/r)^2]+qE_F b\ , \tag{1}$$

$$V_{0,d}=2qEb\ , \tag{2}$$

$$V_{1,s}=Q_e[\varepsilon_1(x/s)+2\varepsilon_2 b(x/s)^2]+qE_F\ , \tag{3}$$

$$V_{1,b}=qE_F\ , \tag{4}$$

$$V_{2,s}=Q_e\varepsilon_2(x/s)^2\ , \tag{5}$$

with $r=\{a,b,c\}$, $s=\{a,c\}$, x as the aluminum molar fraction of Al_xGa_{1-x}As, E_F the intensity of the applied electric field, q the electron charge, Q_e the electron band offset, and m^* the free-electron mass. μ_i (ε_i) are parameters determined by experiments, and associated with the compositional dependence of the electron effective mass (energy gap) of Al_xGa_{1-x}As in the Γ direction.[13] According to Adachi,[13] $\mu_1=0.067$, $\mu_2=0.083$, $\varepsilon_1=1.155$, and $\varepsilon_2=0.37$ at 300 K. The Al_xGa_{1-x}As band-gap energy in the Γ direction is given by $E_g^\Gamma(x)=1.425+1.155x+0.37x^2$.[13]

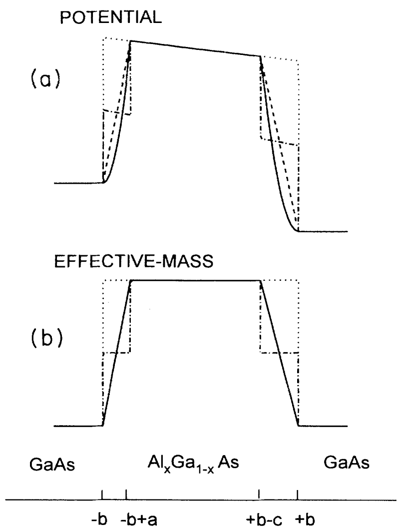

FIG. 1. (a) Potential in a $GaAs/Al_xGa_{1-x}As$ single barrier subjected to an electric field considering abrupt interfaces (dotted line), the LIP approximation obtained from Table I (dashed line), the CIP approximation obtained from Table I (dotted-dashed line), and the complete expressions given in Table I (continuous line); (b) electron effective mass in a $GaAs/Al_xGa_{1-x}As$ single barrier considering abrupt interfaces (dotted line), the CIEM approximation obtained from Table I (dashed line), and the complete expressions given in Table I (continuous line).

Since the potential profiles of abrupt and nonabrupt barriers subjected to an electric field must be identical in the region $-b<z<+b$, where $\mathcal{X}(z)=x$, the abrupt-barrier width $l_A=2b'$ has to be equal to the nonabrupt-barrier width $l_{NA}=2b+a+c$. Consequently, $b<b'$, i.e., the region where $\mathcal{X}(z)=x$ is smaller in the nonabrupt barrier than in the abrupt barrier. This is in contrast to previous definitions of nonabrupt heterostructures.[7,14-20]

The transmission coefficient of an electron through a nonabrupt barrier is calculated by solving the effective-mass equation for the envelope function $\psi(z)$ in all space, with matching conditions imposed on $\psi(z)$ and $[m(z)]^{-1}(d\psi/dz)$ at the borders of the interfaces. The kinetic-energy operator $\mathcal{T}$ has to be modified to describe the spatial dependence of the electron effective mass $m(z)$ in the interfacial regions. The way to include the spatial dependence of the effective mass in $\mathcal{T}$ is not unique, and it is still controversial.[21-23] We choose the following kinetic-energy operator:

TABLE I. Potential and electron effective-mass expressions for a single nonabrupt $GaAs/Al_xGa_{1-x}As$ barrier subjected to an electric field.

Space interval	$V(z)$	$m(z)/m^*$
$z\le -b$	0	μ_1
$-b\le z\le -b+a$	$V_{0,a}+V_{1,a}z+V_{2,a}z^2$	$\mu_1+\mu_2 x(b+z)/a$
$-b+a\le z\le +b-c$	$V_{0,b}+V_{1,b}z$	$\mu_1+\mu_2 x$
$+b-c\le z\le +b$	$V_{0,c}-V_{1,c}z+V_{2,c}z^2$	$\mu_1+\mu_2 x(b-z)/c$
$z\ge +b$	$V_{0,d}$	μ_1

$$\mathcal{T}=(-\hbar^2/2)[(d/dz)m^{-1}(z)(d/dz)] . \quad (6)$$

This operator was originally proposed by BenDaniel and Duke,[24] and it seems to be the most used nowadays. Recently, Liu and Kuhn[17] showed that any kinetic-energy operator could be transformed to that of Eq. (6) with the addition of an effective potential-energy term to $\mathcal{T}$, the form of which depends on the specific spatial dependence of the effective mass.

To study the role of the interfacial description of the potential and effective mass on the transmission properties of electrons through nonabrupt $GaAs/Al_{0.35}Ga_{0.65}As$ single barriers, transmission coefficients are calculated: using the complete spatial dependence of the interface potential and electron effective mass, named T_{pl}; with both the linear interface potential (LIP) and the constant interfacial effective-mass (CIEM) approximation, named T_{lc} (the use of the parabolic interface potential and the CIEM approximation gives practically the same transmission coefficient);[12] with both the constant interface potential (CIP) and the CIEM approximation, named T_{cc}; and with the abrupt picture for the interfaces, named T_{ab}.

The potential and effective-mass approximations are presented in Fig. 1. The effective-mass equations used in the calculations of T_{pl} were solved by applying the multistep method as proposed by Ando and Itoh,[25] while analytical results with the transfer-matrix method were obtained for T_{cc}, T_{lc}, and T_{ab}.[26]

The electron-transmission coefficients T_{pl}, T_{lc}, and T_{cc} of single nonabrupt $GaAs/Al_xGa_{1-x}As$ barriers 100 Å wide, with interfacial widths of 2 and 4 LP, are shown in Figs. 2 and 3, respectively. T_{ab} is also presented for the

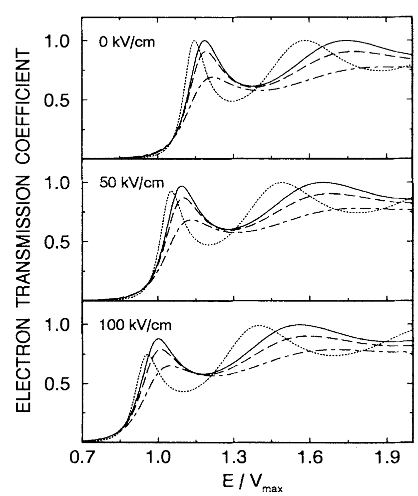

FIG. 2. Transmission coefficients of electrons through single $GaAs/Al_xGa_{1-x}As$ barriers subjected to electric-field intensities of 0, 50, and 100 kV/cm, considering abrupt interfaces (dotted line), the LIP-CIEM approximations obtained from Table I (dashed line), the CIP-CIEM approximations obtained from Table I (dotted-dashed line), and the complete expressions given in Table I (continuous line). A band offset $Q_e=0.6$, an aluminum molar fraction $x=0.35$, and interface widths of 4 LP were used. The abrupt-barrier width was 100 Å.

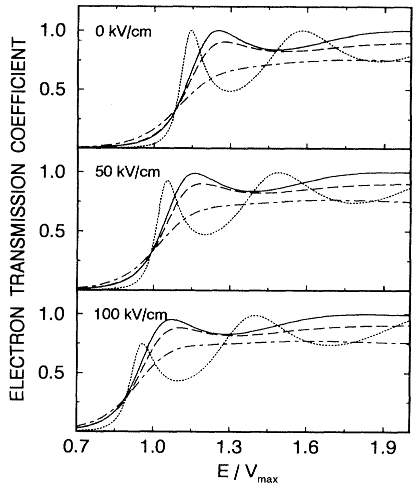

FIG. 3. Transmission coefficients of electrons through single $GaAs/Al_xGa_{1-x}As$ barriers subjected to electric-field intensities of 0, 50, and 100 kV/cm, considering abrupt interfaces (dotted line), the LIP-CIEM approximations obtained from Table I (dashed line), the CIP-CIEM approximations obtained from Table I (dotted-dashed line), and the complete expressions given in Table I (continuous line). A band offset $Q_e = 0.6$, an aluminum molar fraction $x = 0.35$, and interface widths of 2 LP were used. The abrupt-barrier width was 100 Å.

sake of comparison. One could observe that T_{cc} is in general considerably smaller than T_{pl}, T_{lc}, and T_{ab}. T_{cc} does not have peaks of resonance if the interfacial width is bigger or of the order of 4 LP. The resonance peaks (valleys) in T_{pl}, T_{lc}, and T_{cc} are smaller (bigger) and shifted toward high energies in comparison with those of T_{ab}. Consequently, peak-to-valley ratios in the first transmission resonance of nonabrupt single barriers are smaller than those of abrupt barriers. In some cases, the peak-to-valley ratio of T_{pl} (T_{lc}) is smaller compared with that of T_{ab} by as much as 20% (40%) if the interface width is 2 LP, and as much as 40% (60%) if the interface width is 4 LP.

The electric field produces an overall reduction of the electron-transmission coefficient, and shifts the resonance peaks toward low energies. The reduction of the first peak of resonance in T_{pl}, T_{lc}, T_{cc}, and T_{ab} increases with the intensity of the electric field, but is much stronger in the case of T_{ab}. It is interesting to observe that the reduction of T_{pl}, T_{lc}, and T_{cc} with the intensity of the electric field is smaller when the interface is wider. Combined effects due to the electric field and interface widths are less important with the increase of the interface width and/or the intensity of the electric field.

Choi, Newman, and Iafrate[27] presented experimental currents and differential conductance characteristics of a single $GaAs/Al_{0.25}Ga_{0.75}As$ barrier. The fourth resonance peak predicted by them with a theoretical abrupt model is not clearly exhibited in their experimental results. In light of the results obtained here, the existence of an interfacial width as small as 2 LP in the samples used in their experiments could explain this disagreement. On the other hand, the present results suggest that experimental measurements on current-voltage characteristics of heterostructures (see those of Rossel, Guéret, and Meier[28] and Guéret *et al.*[29,30]) are highly dependent of the widths and growth patterns of the sample interfaces.

In conclusion, electron-transmission properties through nonabrupt $GaAs/Al_xGa_{1-x}As$ single barriers subjected to an electric field were presented. It was shown that a good interface representation is necessary to assure better description of the transmission properties of actual samples, whose interface widths are at least of 2 LP. The method used here to describe the interface is totally based on experimental parameters, and seems to be practical and useful as a first approach in the study of nonabrupt $GaAs/Al_xGa_{1-x}As$ heterostructures.

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