Transmission coefficient of electrons through a single graded barrier

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(Received 4 January 1993; revised manuscript received 12 March 1993)

We present a model to describe the effective mass, generalized kinetic-energy operator, and barrier potential to study the motion of an electron across a nonabrupt barrier of GaAs/Al_xGa_{1-x}As/GaAs. With this model, we calculate the transmission coefficient using three different methods. The results obtained with these methods show a significant change of the transmission coefficient when compared with that of an abrupt barrier. Numerical results are obtained for different values of the interfacial width, and compositional variation of the aluminum.

I. INTRODUCTION

The fabrication of high-quality layered semiconductor structures such as quantum wells and potential barriers has allowed the observation of manmade quantum size effects in optical devices.[1,2] In order to obtain the physical properties of such systems, one has to solve the Schrödinger equation involving potentials with complicated profiles. Exact analytical solutions of the Schrödinger equation are available only for simple potential structures such as the square well or the parabolic well. The Schrödinger equation has been solved numerically for an arbitrary potential profile by different methods, such as the multistep potential approximation[3] (MPA), finite element methods[4] (FEM), and the piecewise-linear approximation.[5,6] Using the MPA method,[3] the variations of potential energy and of the electron effective mass are approximated by multistep functions, such that various potential barriers, including continuous variations of potential energy and effective mass, can be analyzed by using this method. With the FEM approach, based on the Galerkin method,[4] the Schrödinger equation is replaced by a system of algebraic equations with parameters that define the approximated solution, and this approach also allows us to treat the effective mass as a continuous function at the interfaces. FEM has been used to calculate the transmission probability through potential barriers[7] and eigenstates in a quantum well.[8] In both methods, MPA and FEM, the boundary condition has the form that the envelope function, and its derivative divided by effective mass, are continuous at the interfaces.

In most of the problems involving heterojunctions, it is assumed that the interface is abrupt.[9,10] However, experimental results have shown the absence of atomically smooth semiconductor heterointerfaces.[11,12] Particularly for the case of GaAs/Al_xGa_{1-x}As, the transition region of the interface can occur from one to two unit cells.[13] It has been observed that the interfacial width and compositional variation considerably change heterostructure properties.[14] Using a nonabrupt potential profile to describe one heterojunction, theoretical calculations have been carried out to analyze the transmission coefficient for electrons and holes.[15,16]

In this paper we study the effects of the interfacial width and compositional variation on the transmission coefficient of electrons across a GaAs/Al_xGa_{1-x}As/GaAs barrier. In Sec. II we present a model to describe the effective mass, generalized kinetic-energy operator, and barrier potential. With this model we calculate the transmission coefficient using three different methods, and in Sec. III we compare the results obtained with these methods as a function of the interfacial width and compositional variation of the aluminum.

II. MODEL DESCRIPTION

The conduction-band energy structure of the system to be studied is a GaAs/Al_xGa_{1-x}As/GaAs barrier with nonabrupt interfaces, as shown in Fig. 1, and under the effective-mass approximation, the envelope function of the electron is given by a one-dimensional time-independent Schrödinger equation. We assume that the aluminum molar fraction χ changes linearly at the transition regions, such that it can be written as

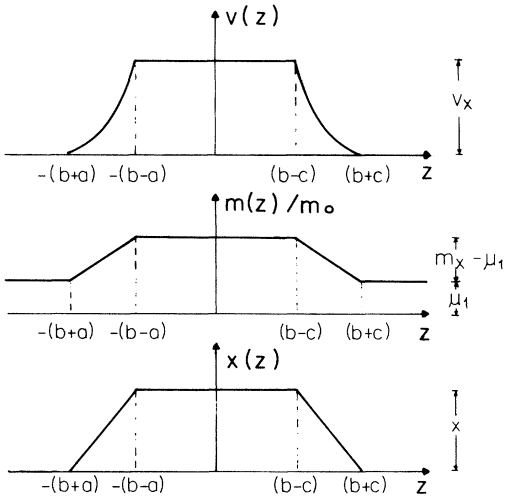

FIG. 1. Potential barrier, effective mass, and the aluminum molar fraction, as a function of the position.

$$\chi(z)=\begin{cases}0\ , & z<-(b+a)\\ (x/2a)(z+b+a)\ , & -(b+a)<z<-(b-a)\\ x\ , & -(b-a)<z<(b-c)\\ (x/2c)(b+c-z)\ , & (b-c)<z<(b+c)\\ 0\ , & z>(b+c)\ ,\end{cases} \tag{2.1}$$

where $2b$ is the barrier width and x is the $Al_xGa_{1-x}As$ aluminum molar fraction. The transition regions occur from GaAs to $Al_xGa_{1-x}As$ between $z=-(b+a)$ and $z=-(b-a)$ and from $Al_xGa_{1-x}As$ to GaAs between $z=(b-c)$ and $z=(b+c)$, respectively. By considering that the $Al_xGa_{1-x}As$ conduction-band energy-band-structure dependence on x is valid for angstrom dimensions,[17] the potential that determines the electron motion in space, as shown in Fig. 1, is given by

$$V(z)=C[\epsilon_1\chi(z)+\epsilon_2\chi(z)^2]\ , \tag{2.2}$$

where C is the band offset and ϵ_1,ϵ_2 are constants associated with the compositional dependence of the energy-gap difference between $Al_xGa_{1-x}As$ and GaAs.[17]

The electron's motion across the barrier is described by a Hamiltonian with a kinetic-energy operator having a position-dependent effective mass, as proposed by von Ross,[18] that is,

$$\hat{T}=\tfrac{1}{4}(m^{\alpha}\hat{p}m^{\beta}\hat{p}m^{\gamma}+m^{\gamma}\hat{p}m^{\beta}\hat{p}m^{\alpha})\ , \tag{2.3}$$

with $\alpha+\gamma+\beta=-1$, $\hat{p}$ is the momentum operator, and m is the effective mass. Since the effective mass in the $Al_xGa_{1-x}As$ is proportional to the aluminum concentration,[17] we assume that for the system under consideration this is also true at the transition regions. With this assumption, the effective mass changes continuously according to

$$\frac{m(z)}{m_0}=\mu_1+\mu_2\chi(z)\ , \tag{2.4}$$

where μ_1,μ_2 are parameters obtained experimentally[17] and m_0 is the free-electron mass. The generalized boundary conditions used by Morrow and Brownstein[19] will be considered.

In order to obtain the transmission coefficient of the electrons through a graded barrier, we use three different methods. In the first one we assume a constant effective mass (CEM) across the transition region, as used by Freire, Farias, and Auto.[15] In this approximation, at the transition region, the effective mass is the average value between its value in the GaAs and $Al_xGa_{1-x}As$, and the potential is a linear function of z. In the second method we use the multistep potential approximation[3] and finally we apply the finite element method.[4]

III. RESULTS AND DISCUSSION

In order to obtain numerical results, we use the experimental parameters given in Ref. 17 and consider the band offset equal to 0.6. To compare all approximations, we assume for the kinetic operator, Eq. (2.3), $\alpha=\gamma=0$ and $\beta=-1$. In all cases we observed that when the MPA and FEM approaches converge, they give the same results for the transmission coefficient of the electrons through the barrier. The convergence of the MPA approach was obtained by dividing each transition region of the barrier into $N=30$ intervals, while to obtain the same result using FEM it was necessary to consider $N=25$ for the whole region of the barrier. Since both methods give the same results, we will plot the transmission coefficient of the electron using the MPA approach, because MPA take less computer time than FEM.

From the result obtained we observed that the existence of a transition region in a barrier decreases the amplitude of oscillation of the transmission coefficient, which is consistent with experimental results reported by Kim and Arnold.[20]

Using all the approximations, in Fig. 2 we show the transmission coefficient of electrons on abrupt and nonabrupt barriers of width 100 Å, aluminum molar concentration $x=0.35$, and a symmetric transition region of widths $l=2a=2.0$, 4.0, 6.0 LP, where LP is the lattice parameter of GaAs. We first observe that for all values of l, the peak-to-valley ratio (PVR) in the abrupt barrier is greater than those obtained by assuming a nonabrupt interface. As the transition region increases, the PVR decreases, and the peaks shift toward high energies.

In Fig. 3 we plot the transmission coefficient of elec-

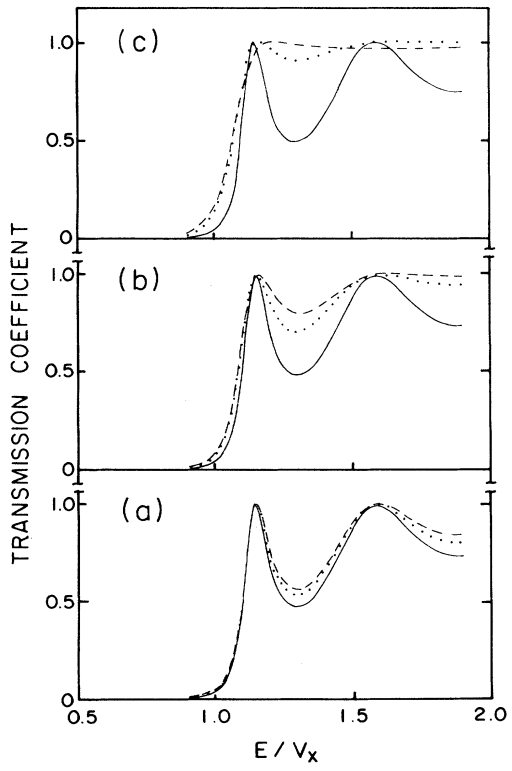

FIG. 2. Transmission coefficient as a function of the incident electron energy, for a barrier of width 100 Å, aluminum concentration $x=0.35$, and a symmetric transition region of (a) 2.0, (b) 4.0, and (c) 6.0 LP: abrupt barrier (——), the CEM method (— — —), and the MPA method (· · · ·).

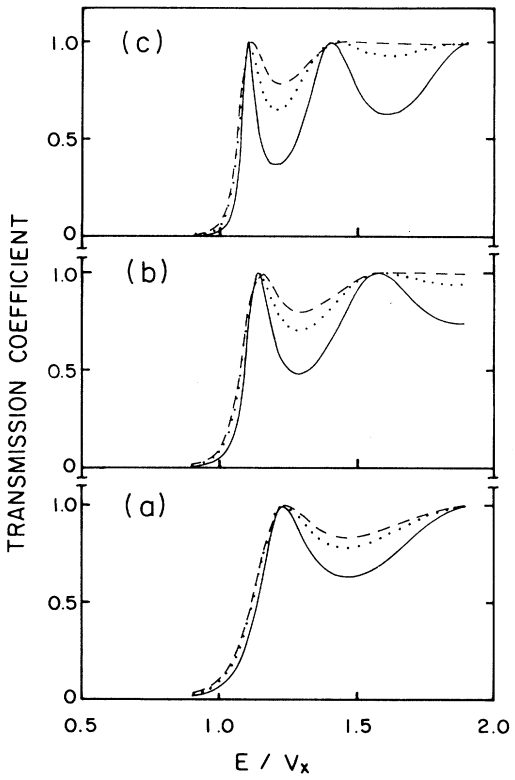

FIG. 3. Transmission coefficient as a function of the incident electron energy, for a barrier of width 100 Å, a symmetric transition region $l=2a=4.0$ LP, and an aluminum concentration of (a) 0.25, (b) 0.35, and (c) 0.45: abrupt barrier (——), the CEM method (— — —), and the MPA method (· · · ·).

trons on abrupt and nonabrupt barriers of width 100 Å, for a symmetric transition region of width $l=2a=4.0$ LP, and with an aluminum molar concentration of $x=0.25$, 0.35, and 0.45. When the aluminum concentration decreases, we note that the difference between the results obtained for abrupt and nonabrupt barriers became small. This result is due to the fact that the barrier potential depends on the aluminum concentration; consequently, the charge in the effective mass is less significant for small concentrations. Again, we observe that for all values of the aluminum concentration x, the peak-to-valley ratio in the abrupt barrier is greater than those obtained by assuming a nonabrupt interface. For the same value of the aluminum concentration, we note that there is no shift of the peaks to high energies when we compare abrupt and nonabrupt barriers.

In Fig. 4 we analyze the effect of the symmetry on the transition region by considering a barrier of width 100 Å, an aluminum molar concentration of $x=0.45$, and transition regions of $a=c=2.0$ LP, and $a=1.0$ LP, $c=3.0$ LP. We observe that the PVR is greater in the barrier with a symmetric transition than in the unsymmetric one. Furthermore, we note that the transmission coefficient does not change in the unsymmetric barrier, when we invert the values of a and c.

In Fig. 5 we present the transmission coefficient considering $\beta=0,-1$ in the kinetic-energy operator. In Fig. 5(a) we consider an abrupt barrier with $l=100$ Å and $x=0.35$. As can be seen, there is a significant change in the transmission coefficient due to the boundary conditions.[19] In Fig. 5(b) we present the transmission coefficient for a nonabrupt barrier of width $l=100$ Å, $x=0.35$, and $a=c=3.0$ LP. Since the effective mass changes smoothly from one region to another, we note that the difference between the results is smaller when compared with the abrupt barrier. Although most previous work assumes $\beta=-1$, we believe that experimental results are necessary to establish the correct value of β.

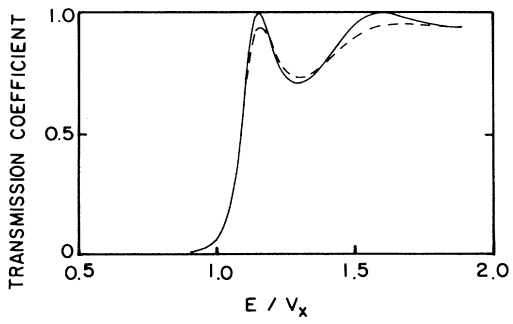

FIG. 4. Transmission coefficient as a function of the incident electron energy, for a barrier of width 100 Å, aluminum concentration $x=0.35$, using the MPA method: asymmetric transition region with $a=c=2.0$ LP (——) and an unsymmetric transition region with $a=1.0$ LP and $c=2.0$ LP (— — —).

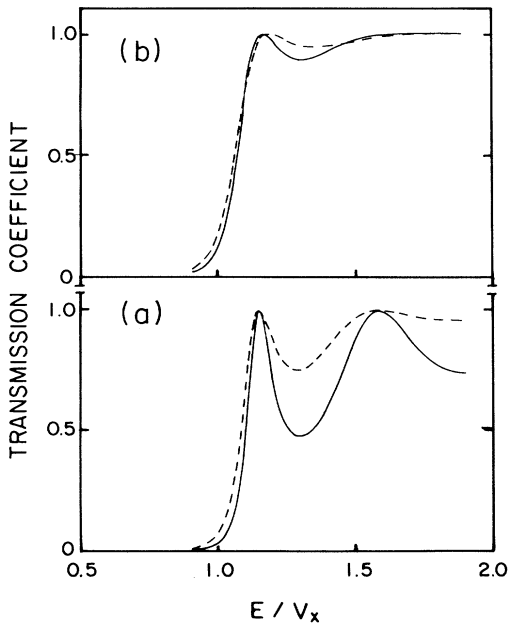

FIG. 5. Transmission coefficient as a function of the incident electron energy, for a barrier of width 100 Å, aluminum concentration $x=0.35$, with $\beta=0$ (— — —) and $\beta=-1$ (——), for an abrupt barrier (a) and a nonabrupt barrier (b), with a symmetric transition region of $l=2a=6.0$ LP.

In conclusion, the effect of a transition region on the transmission coefficient of electrons through a barrier of less than 200 Å is significant. Since the MPA and FEM approaches consider the effective mass to be changing continuously, they represent a more realistic method to describe a nonabrupt barrier when compared with the CEM approach. We are now analyzing the effect of the transition region on resonant tunneling through a double barrier.

ACKNOWLEDGMENTS

This work was supported in part by CNPq and FINEP.

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