Armenian Journal of Physics, 2011, vol. 4, issue 4, pp. 211-220

EFFECT OF INTERDIFFUSION AND ELECTRIC FIELD ON RESONANT STATES AND CURRENT-VOLTAGE CHARACTERISTIC OF GaAs/$Al_xGa_{1-x}As$ DOUBLE-BARRIER RESONANT STRUCTURE

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Received 17 July, 2011

Abstract–The effect of interdiffusion and electric field on resonant states and current-voltage characteristic in GaAs/$Al_xGa_{1-x}As$ double-barrier structure is investigated. The Schrödinger equation is solved in the complex energy approach and the resonance energies, as well as the corresponding wave functions are obtained. The dependences of the resonance energies and the resonant current density on the electric field strength for different values of diffusion length and temperature are obtained. It is shown that for certain values of diffusion length and electric field strength the appearance of quasibound states of second type and the conversion of a number of quasibound states of first type to corresponding states of second type are possible. It is also shown that at lower temperatures interdiffusion leads to the weakening of the effect of electric field on the resonant current density while at room temperature the effect of electric field becomes stronger due to interdiffusion.

Keywords: double-barrier resonant structure, interdiffusion, electric field, resonance current

1. Introduction

The artificially grown crystals, known as one-dimensional superlattice nanostructures, nanodevices, mesoscopic devices, and semiconductor heterostructures, are composed of alternating layers of different semiconductor materials with nanometer thickness (see, e.g., [1]). For electrons and holes they represent a one-dimensional alternating sequence of potential wells and barriers. In principle, the properties of mentioned nanosystems can be changed at will by adjusting the chemical composition and thickness of the layers, i.e., by constructing a given potential profile, to suit specific applications.

Over the last several years the subject of resonant tunnelling has became an area of detailed study [2-9] partly due to its importance in areas like nanoscience and electronic devices. In general, in non-relativistic quantum mechanics the resonance phenomena can be related to the comparatively long-lived positive energy states. When they have very narrow widths, they are often referred to as quasi-bound states (QBS).

Analytic *S*-matrix (SM) theory of potential scattering [10-16] provides a unified picture of bound states and resonances in terms of the pole structure of partial wave SM.

Several methods for locating the bound states and resonances generated by one-dimensional potentials have been developed over the past decades (for references and review of the existing methods, see [17]). Practically all of them are based on the so-called transfer-matrix approach.

Undoubtedly, the transfer-matrix approach is relatively simple and rather universal although it is not suitable in some cases. For example, it is difficult to use the transfer matrix when the potential has slowly decaying tails outside the physical structure (for instance, when charge is accumulated on the surfaces) and one has to go too far to achieve convergence of the results. The rectangular discretization is also not satisfactory when the potential profile has segments of fast variations (near impurities, for instance) or is biased by a strong electric field (Stark effect) [18].

In [6] an exact and unified method which belongs to the category of complex-energy approaches was developed for solving the one-dimensional Schrödinger equation on an infinite line at any complex energy for an arbitrary potential profile. This method is very efficient and accurate in locating not only bound states and narrow resonances but extremely wide and overlapping resonances as well.

At this point it should be noted that the motion of a particle on an infinite line is inherently a multichannel problem that has at least two channels involved. These two channels are the motion on the left and right halves of the line. If the resonance energy is larger than both the left and the right asymptotes of the potential energy, the resonant state can decay into both channels (both directions), otherwise it can decay only into one of them. Sometimes these two types of resonances are called QBS of the first and second type, respectively [17].

In this work the effect of interdiffusion and electric field on resonant states and current-voltage characteristic in a double-barrier structure is investigated. The Schrödinger equation is solved in the complex energy approach. It is shown that the existence of QBS of the first or the second type depends on the electric field strength and the diffusion length. The dependences of the resonance energies and the resonance current density on the electric field strength for different values of diffusion length and temperature are obtained as well.

2. Theory

We consider a GaAs/$Al_xGa_{1-x}As$ double-barrier structure consisting of a well of width a surrounded by two barriers of widths b_1 and b_2 with the same height. The center of the well is assumed to be coincided with the origin of *z*-axis which is the growth direction. This structure is subjected to an external electric field $\mathbf{F}$ directed oppositely to the *z*-axis and applied in the region $[-a_0, a_0]$. The potential profile of considered system in the absence of electric field is defined by the distribution of Al concentration x as follows:

$$V(z;L) = Q_e B x(z;L), \tag{1}$$

where L is the diffusion length, $Q_e = 0.6$ is the band offset coefficient for GaAs and $B = 1.247$ eV. The concentration profile $x(z;L)$ can be obtained from the Fick's law [19] by the assumption that before the diffusion process the atoms of Al are concentrated only in the barrier regions with the constant concentration $x(z;0) = x_0$. After simple transformations and taking into account the effect of electric field one can arrive to the following expression for the potential profile:

$$V(z) = \Theta(a_0 - |z|)[eFa_0 + V_d(z) - eFz] + \Theta(-a_0 - z)2eFa_0, \tag{2}$$

where $\Theta(z)$ is the unit step function, *e* is the magnitude of the electron charge,

$$V_d(z) = \frac{V_0}{2}\left[erf\left(\frac{z + \frac{a}{2} + b_1}{L}\right) - erf\left(\frac{z + \frac{a}{2}}{L}\right)\right] + \frac{V_0}{2}\left[erf\left(\frac{z - \frac{a}{2}}{L}\right) - erf\left(\frac{z - \frac{a}{2} - b_2}{L}\right)\right] \tag{3}$$

is the potential profile formed after the interdiffusion in the absence of electric field, V_0 is the height of barriers before interdiffusion [20], $erf(x)$ is the error function [21].

Figure 1 illustrates the dependence of this potential (in units of the Rydberg energy: $E_R = 5.2$ meV) on the dimensionless (in units of the effective Bohr radius $a_B = 104$ Å) *z*-coordinate for different values of diffusion length when the dimensionless electric field strength $f \equiv eFa_B/E_R = 0.3$ (note that for GaAs the value $f = 1$ corresponds to $F = 5$ kV cm^{-1}).

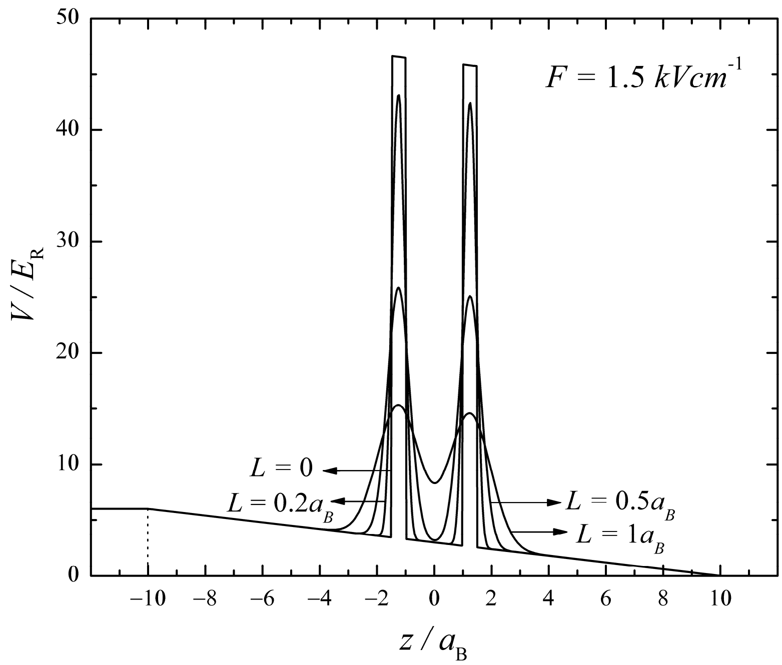

Fig. 1. Dependence of the double-barrier confining potential in the electric field on the dimensionless coordinate in growth direction ($a_0 = 10a_B$).

The wave functions (WF) of resonance states $\Psi(E_{res}, z)$ with the energy E_{res} obeys the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(E,z)}{\partial z^2} + V(z)\Psi(E,z) = E\Psi(E,z) \tag{4}$$

and the boundary conditions [6]

$$\begin{aligned} A_L^{(-)} e^{-ik_L z} \leftarrow_{z=-a_0} \Psi(E_{res}, z)_{z=a_0} \rightarrow A_R^{(+)} e^{ik_R z}, \\ -ik_L A_L^{(-)} e^{-ik_L z} \leftarrow_{z=-a_0} \Psi'(E_{res}, z)_{z=a_0} \rightarrow ik_R A_R^{(+)} e^{ik_R z}, \end{aligned} \tag{5}$$

where $A_{L(R)}^{(-)}$ is asymptotic normalization constant, $k_{L(R)} = \sqrt{2m\left(E_{res} - V_{L(R)}\right)/\hbar^2}$ is the wave vector in the region $(-\infty, -a_0]$ ($[a_0, \infty)$), m is the effective mass of electron and, according to Eq. (2), $V_L = 2eFa_0$, $V_R = 0$. The conditions (5) provide that there are only outgoing waves outside the resonant structure. The solutions of this kind exist at complex values of energy $E_{res} = E_r + iE_i$ with the imaginary part E_i that describes the characteristic width of the corresponding energy level Γ ($|E_i| = \Gamma/2$). It should be noted that if $E_r \geq 2eFa_0$ then E_i is negative and the resonant WF can decay into both directions (QBS of the first type), otherwise E_i is positive and WF can decay only into the right direction (QBS of the second type).

Since Eq. (4) is of the second order, its fundamental system of solutions consists of any two linearly independent functions obeying this equation. This two functions $\phi_1(E,z)$ and $\phi_2(E,z)$ can be obtained by the shooting method with the following requirements on their values at $z=0$ (symmetric and antisymmetric solutions):

$$\phi_1(E,0) = 0,\ \phi_1'(E,0) = 1, \tag{6}$$

$$\phi_2(E,0) = 1,\ \phi_2'(E,0) = 0. \tag{7}$$

Since the Wronskian of any two solutions of Eq. (4) is independent of z, we can calculate it at $z=0$. Hence $W(\phi_1,\phi_2) = -1$ for all points of interval $(-\infty, +\infty)$, which means that the conditions (6) and (7) guarantee the linear independence of the basic solutions ϕ_1 and ϕ_2. Any physical solution $\Psi(E,z)$ of Eq. (4) is a linear combination of the basic solutions

$$\Psi(E,z) = C_1\phi_1(E,z) + C_2\phi_2(E,z). \tag{8}$$

By imposing the boundary conditions (5) on the WF (8), one can obtain a system of linear algebraic equations for C_1, C_2, $A_L^{(-)}$ and $A_R^{(+)}$ which has a nontrivial solution when its determinant equals zero:

$$\begin{vmatrix} \phi_1(E,a_0) & \phi_2(E,a_0) & -e^{ik_R a_0} & 0 \\ \phi_1'(E,a_0) & \phi_2'(E,a_0) & -ik_R e^{ik_R a_0} & 0 \\ \phi_1(E,-a_0) & \phi_2(E,-a_0) & 0 & -e^{ik_L a_0} \\ \phi_1'(E,-a_0) & \phi_2'(E,-a_0) & 0 & ik_L e^{ik_L a_0} \end{vmatrix} = 0. \tag{9}$$

We develop a numerical procedure based on the bisection method for obtaining the complex values of energy which satisfy equation (9).

The current density is calculated from the following expression [2]:

$$J(T) = -\frac{emk_B T}{2\pi^2\hbar^3}\int_0^\infty T(E_\perp)\ln\left\{\frac{\left(1+\exp\left[\dfrac{\mu(T)-E_\perp}{k_B T}\right]\right)}{\left(1+\exp\left[\dfrac{\mu(T)-E_\perp+2eFa_0}{k_B T}\right]\right)}\right\}dE_\perp, \qquad (10)$$

where k_B is the Boltzmann constant, T is the absolute temperature, $E_\perp$ is the energy of motion in the *z*-direction, $T(E_\perp)$ is the transition probability that can be replaced by Lorentzian function as is shown in [22] and $\mu(T)$ is the chemical potential which is obtained from the condition of being constant of the electron concentration in the conduction band [23].

3. Discussion

Our calculations are done for a double-barrier structure consisting of a GaAs well sandwiched between two $Al_{0.3}Ga_{0.7}As$ barriers for different values of diffusion length and temperature. The initial widths of the well and barriers are taken to be $a = 2a_B$, $b_1 = b_2 = 0.5a_B$ respectively, and $a_0 = 10a_B$.

As seen from Fig. 1, the intermixing of Al and Ga atoms initially concentrated in the barriers and the well region results in two main changes in the potential profile: the smearing of initially rectangular potential and the reduction of the well's depth and barriers' height. Moreover, as a result of the electric field effect an additional triangular-like well appears in the region $z \in [-10a_B, -1.5a_B]$, where QBS of the second type can exist.

In Fig. 2 the dependences of resonant energies on the electric field strength for different values of diffusion length are presented. One can see from the figure that in the case of $f = 0$ there are only QBS of the first type. With increase in f a QBS of the second type appears in the region $z \in [-10a_B, -1.5a_B]$. In the cases of $L = 0$ and $L = 0.2a_B$ for the value of electric field strength $f \simeq 0.186$, the first QBS of the first type converts to the second QBS of the second type in triangular-like well. Starting from a certain value of f ($f \simeq 0.3$ for the values of $L = 0$ and $L = 0.2a_B$ and $f \simeq 0.355$ for $L = 0.5a_B$) the third QB state of second type appears. It is noticeable that for $L = 0.5a_B$ (Fig.2c) the first QBS of the first type exists for $f \le 0.355.$. In this case the conversion from the first QBS of the first type to the third QBS of the second type takes place in contrast to the cases of $L = 0$ and $L = 0.2a_B$. It is because of the rising up of the QBS energy levels and the weakening of quantum confinement effect due to interdiffusion, which causes the increase in the minimal value of f that is necessary for confining the first QBS of the first type. One can also see that the increase in f causes the almost linear increase in the energies of both types of states and the dependence on the electric field is stronger for QBS of the second type. Comparing Figs. 2*a*, *b* and *c*, one can observe that by increasing the diffusion length, the energies of all resonant states increase due to rising of the bottom of the well and QB states of first type are more sensible with respect to interdiffusion because of their weaker confinement.

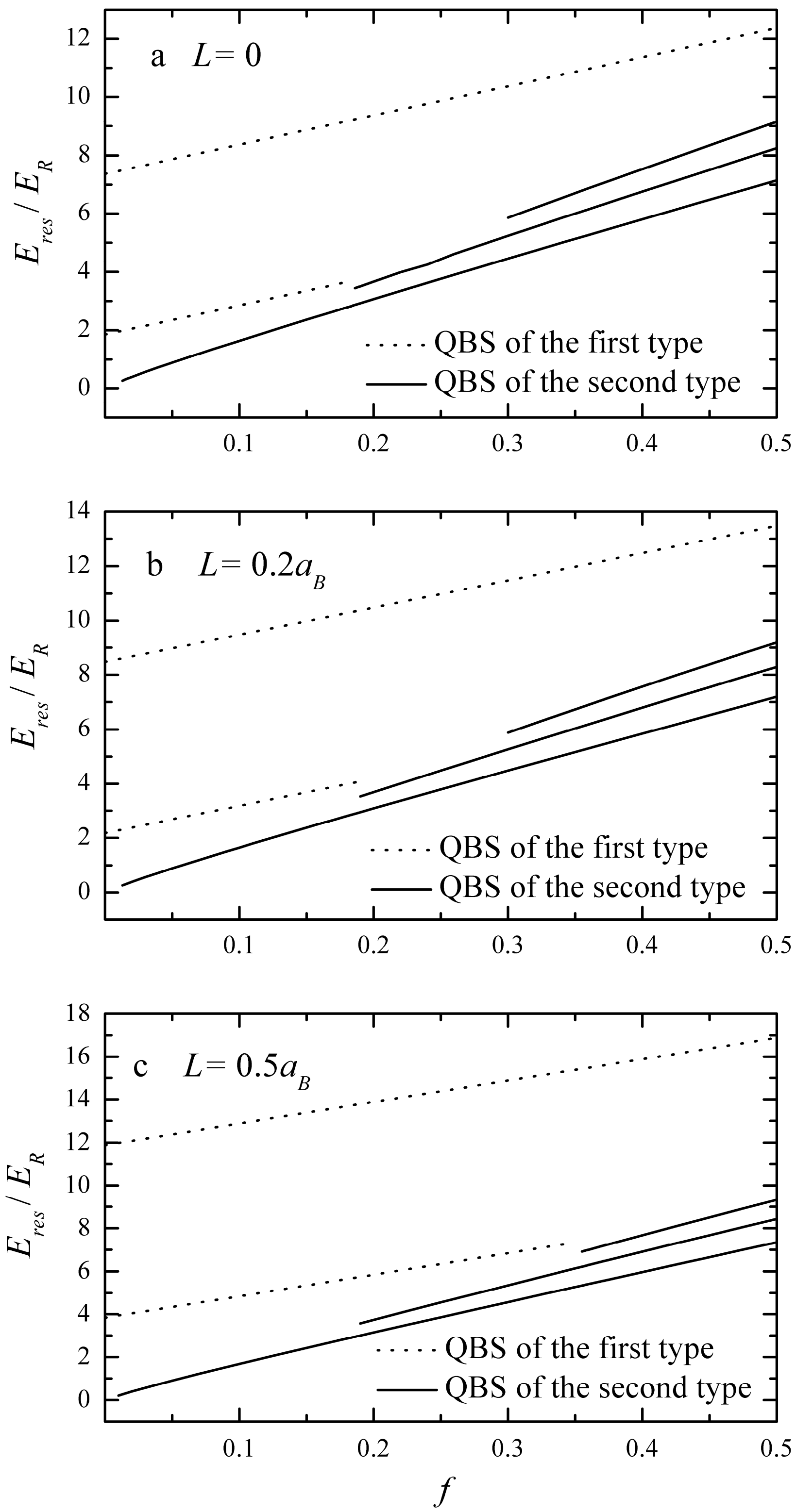

Fig. 2. Dependence of the resonant state energies on the dimensionless electric field strength.

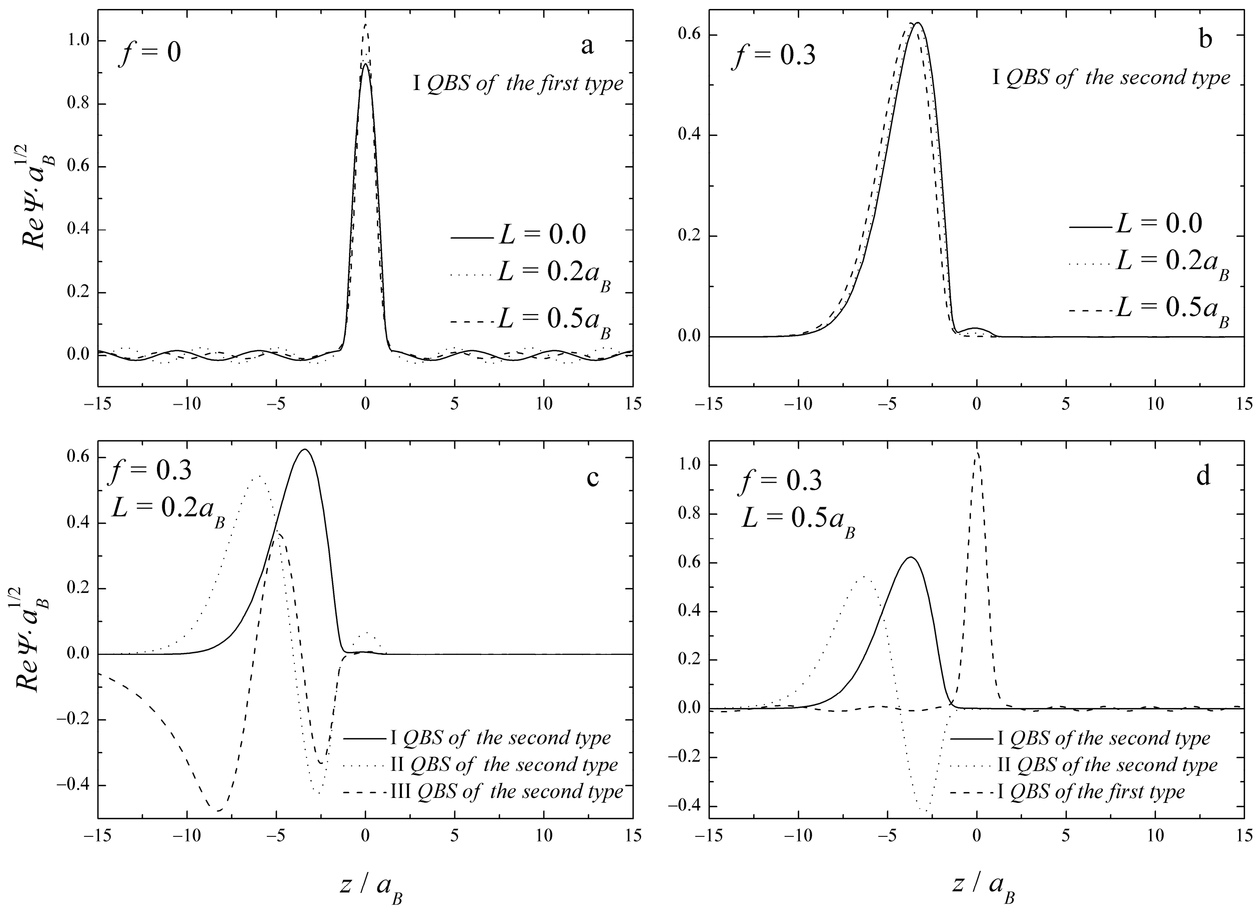

Fig. 3. Dependences of the resonant state wave function on the coordinate in growth direction.

In Fig. 3 the dependences of the real part of QBS WF on the *z*-coordinate are presented. In Fig. 3*a* the WF of the first QBS is shown for different values of diffusion length in the case of $f = 0$. In this case only the QBS of the first type are possible. As seen from the figure, the WF has a strong maximum in the center of the well between the barriers and has weak oscillations in the left and right regions which are extended to infinity. By increasing the diffusion length, the value of the maximum increases because of the widening of the barriers in their lower part, where the first QBS is located. The oscillations frequency becomes larger due to the increase in resonant energies and the quasi-momentum of charge carriers. In Fig. 3*b*, the same dependence is shown for the first QBS of the second type in the case of $f = 0.3$. As it was mentioned above, this WF is mostly located in the region of the triangular-like well. For smaller values of L ($L = 0$ and $L = 0.2a_B$) there is also a very small peak in the center of well between barriers (further we will call it the "main well") due to tunnelling effect through the left barrier. By increasing the diffusion length the smaller peak disappears (the effective width of the left barrier for this state becomes larger) and the larger one shifts to the left (the smearing leads to the shift of the bottom of triangular-like well to the left. Figs. 3*c* and 3*d* illustrate the WFs of the three lowest QBS for two different values of diffusion length when $f = 0.3$. For $L = 0.2a_B$ (Fig. 3*c*) these WFs are like the WFs of the ground, first and second excited states in a quantum well in the region $z \in [-10a_B, -1.5a_B]$. However, for $L = 0.5a_B$ (Fig. 3*d*) the WF of the third QBS has a different character comparing with the case of $L = 0.2a_B$. This is a QBS of the first type, while the first and second states are QBS of the second type. The small peak in the "main well" is evident for smaller values of L because of a bit stronger tunneling through the left barrier. In Fig. 3*c* the value of this peak for the third QBS is smaller than the peak for the second one. This is because of the stronger tunneling of the third QBS through the right barrier. For $L = 0.5a_B$. practically there is no any probability of being electron in the "main well" for QBS of the second type (solid and dotted lines in Fig. 3*d*) and only QBS of the first type can tunnel through the resonant structure. It is noteworthy that the wavelength of the WF of this state is smaller in the region $z \in [1.5a_B, 10a_B]$ due to the larger value of $E - V(z)$ comparing with the region $z \in \left[-10a_B, -1.5a_B\right]$.

In Fig. 4 the dependences of the resonant current density (in units of $J_0 = 296.42$ A/mm^2) on the electric field strength for different values of the diffusion length and temperature are presented. It is clear that for all values of diffusion length, the increase in f leads to an initial increase the current density almost linearly and then to its sharp drop to a very small value (of the order of 10^{-6}) which is related to the fact that the lower QBS of the first type is substituted by a second type one. It is necessary to mention that in comparison with the QBS of the first type, the second type states make a negligible contribution in the current density because of their negligibly small energy width. With the increase in f the initial increase in the current density occurs slower for larger values of diffusion length due to weaker tunnelling of electrons through the barriers that becomes wider for first QBS of the first type. After the sharp drop in the current density, which takes place with the disappearance of this state, the curves have a nonlinear behavior. This fact is caused by the increase in the Fermi–Dirac distribution function in the second QBS of the first type starting from approximately zero value (the chemical potential is much smaller than the energy of this state for any values of temperature) in the region $(-\infty, -a_0]$ and by its decrease in the region $[a_0, \infty)$. For larger values of L this process starts from the larger value of f (dotted and dash-dotted curves in Fig. 4a and Fig. 4b). Note that a sharp drop of the current density for $L = 0.5a_B$ occurs at $f \simeq 0.355$ (in contrast to the cases of $L = 0$ and $L = 0.2a_B$ for which this drop occurs at $f \simeq 0.185$), because the first QBS of the first type does not disappear until this value of f. Comparing Figs. 4*a*, 4*b*, and 4*c*, one can observe that the increase in the temperature results in the increase in the current density for any values of L and f because of the larger contribution of higher resonances. As a result the sharp drops for $T = 200K$ are insignificant in comparison with the values of current density. In addition, the temperature effect on the current density is more significant for $L = 0.5a_B$, which is explained by larger width of the second QBS of the first type, the contribution of which becomes larger at high temperatures due to increase in the Fermi–Dirac distribution function. Eventually for $T = 300$ K which is not shown in figures, the current density varies almost linearly with f with the negligible sharp drop for any values of the diffusion length and electric field strength.

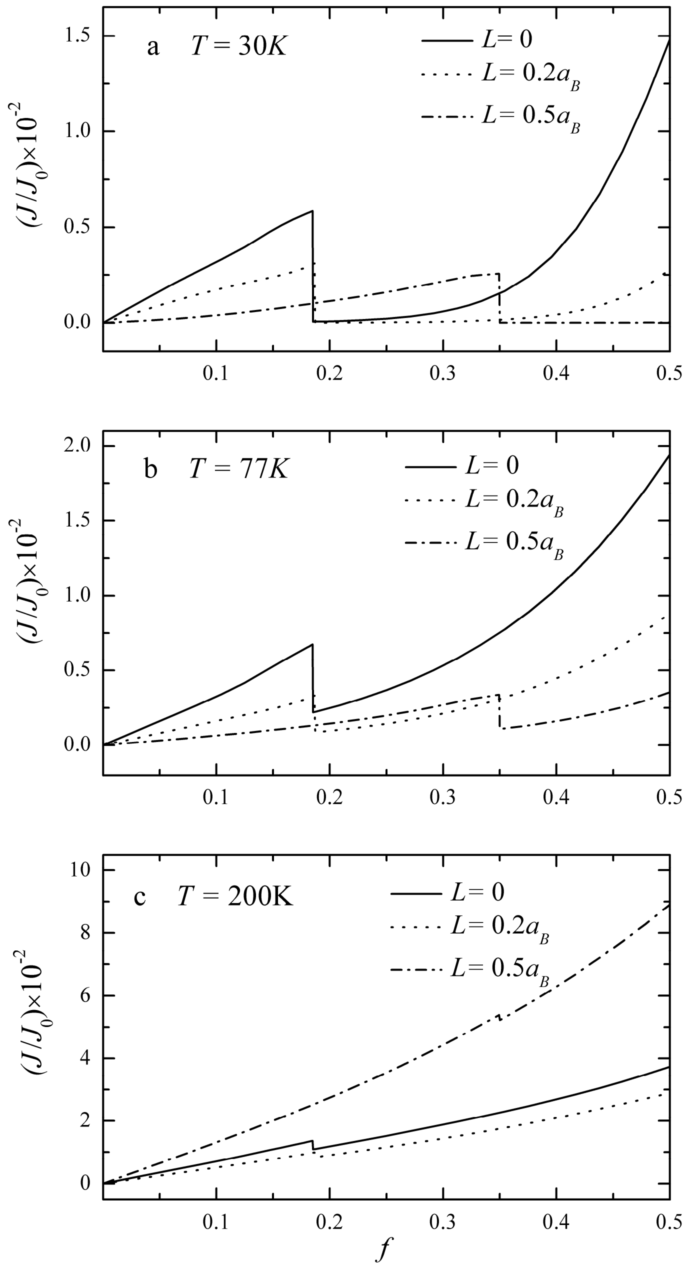

Fig. 4. Dependence of the resonant current density on the dimensionless electric field strength.

4. Conclusion

Summarizing, the effect of interdiffusion and electric field on resonant states and current-voltage characteristic in GaAs/$Ga_{1-x}Al_xAs$ double-barrier structure is considered. The Schrödinger equation is solved in the complex energy approach using the shooting method. The resonance energies, as well as the corresponding wave functions are obtained. The dependences of the resonance current density on the electric field strength for different values of the diffusion length and temperature are studied. It is shown that for certain values of the diffusion length and electric field strength, it is possible the appearance of QBS of the second type and the conversion of a number of QBS of the first type to corresponding states of the second type. It is also shown that at lower temperatures interdiffusion leads to the weakening of the effect of electric field on the resonant current density while at higher temperatures the effect of electric field is stronger for large values of the diffusion length. Our results indicate on the possibility of manipulation of the QBS and the main properties of the current–voltage characteristic of the double-barrier resonant structure by means of interdiffusion.

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