Localized states in the barrier of superlattices

S. Erkoc and S. Ciraci
Department of Physics, Middle East Technical University, 06531 Ankara, Turkey
(Received 6 February 1986)

Recent studies have revealed that the so-called confined resonance states with energy above the barrier but localized in the barrier material occur in multiple-quantum-well structures. In this study we carry out self-consistent calculations of the confined and itinerant electron states of a GaAs-$Ga_{1-x}Al_xAs$ superlattice within the effective-mass theory. We show that the modifications of the quantum well due to the Coulombic interactions among electrons and ionized donors cause the localized states to form in the barrier potential. These states are expected to influence the transport properties.

Recent developments in molecular-beam epitaxy as a technique for the growth of ultrathin layers of highly perfect crystals have made the production of superlattices possible.[1] Semiconductor superlattices or multiple-quantum-well structures consist of alternating layers of semiconducting single crystals whose electronic properties, in particular band gaps, are different. Within the effective-mass approximation a GaAs-$Ga_{1-x}Al_xAs$ superlattice can be described by multiple potential wells of the GaAs region which are separated by the $Ga_{1-x}Al_xAs$ barrier as high as the conduction- (valence-) band discontinuity. Electrons (or holes) confined in these one-dimensional wells provide a new regime of quantum effects.[2] In the past the well-confined states have been extensively studied. Theoretically, conventional band-structure methods[3,4] with moderately large supercells, and envelope-function methods,[5] have provided results in reasonable agreement with the experimental observations. However, some important aspects of the problem could not been taken into consideration in these theoretical methods. For example, in spite of the fact that the discontinuities in the potential and thus in the band gaps are indigenous, and the confined states with multivalley interactions are directly obtainable, the self-consistent electronic band-structure caluclations via large supercells seem to be rather difficult. On the other hand, investigations by using the envelope function and also by the effective-mass approximation are simple enough to see fundamental aspects of the quantum-well states. Even for these simple methods of calculations the self-consistency, particularly the screening of the confined electrons, becomes very crucial for a correct description of the quantum-well states.

In this paper we aim to show that self-consistency, especially of the potential due to the excess charged particles (electrons, holes, and ionized impurity atoms) in a doped superlattice is important not only for well states, but also for resonance states confined in the barrier region. Here we start with a brief review of these localized states, which are important for the transport properties of superlattice structures. Using the empirical pseudopotential calculations Jaros, Wong, and Gell[4] have recently reported a new localized state with a large amplitude above the barrier. They proposed that the Γ states of $Ga_{1-x}Al_xAs$ crystals are forced to form wave packets in this region of the semiconductor because of the virtual barrier created by the absence of higher energies of suitable matching partners in the GaAs layers. The fact that not only the band-structure methods but also other simple methods, for example, the effective-mass approximation, are capable of yielding the confined resonance states (CRS's) becomes evident by the work of Weaire and Kermode.[6] They pointed out that the presence of bound (confined well) states at lower energies causes, via the requirement of orthogonalization, a strong reduction in the amplitude of higher states in the well region. Bastard *et al.*[7] also reported the presence of a similar kind of hole state which was named the virtual bound hole state. They explain the origin of localization as due to the repulsion by the quantum well.

In this study we report a rather elusive and novel result and show that the CRS's normally localized in the $Ga_{1-x}Al_xAs$ region may also occur in the original barrier potential determined by the conduction-band discontinuity. We carried out calculations for the excess electron states of the GaAs-$Ga_{1-x}Al_xAs$ superlattice within the effective-mass theory. By assuming a free-electron behavior in the xy plane we solved the one-dimensional Schrödinger equation in the z direction self-consistently. Here the periodic potential $V(z)$ contains the Coulomb potentials of the ionized electrons and donor ions and the exchange potential as well. Positively charged donor ions are treated within the jellium model. In the solutions we assumed that self-consistency is reached when the difference in energy eigenvalues and potentials are within a preset value ($\sim 10^{-4}$ a.u.). The parameters of the superlattice, such as the height of the barrier, V_0 (which is, in fact, a function of the Al concentration), the widths of the well and barrier, d_1 and d_2, and the level of doping were taken from the work of Mori and Ando[8] who used the expansion method. This way we were able to compare our results regarding the confined states with their results, and obtain excellent agreement therefrom.

Considering the central point difference methods the periodic one-dimensional Schrödinger equation is reduced to a recursion relation.

$$\alpha\Psi_{i-1}+(\beta-\lambda)\Psi_i+\alpha^*\Psi_{i+1}=0\,,$$

where $\Psi_i = \Psi(k_z, z_i)$ is the periodic part of the Bloch wave in the z direction

$$\alpha = -\frac{\hbar^2}{2m^*}\left(1 - i\frac{2\pi k_z}{d}\delta\right),$$

$$\beta = \frac{\hbar^2}{2m^*}\left(2 + \frac{4\pi k_z^2}{d^2}\delta^2\right) + \delta^2 V(z_i),$$

and $\lambda = \delta^2 E_n$. In these equations δ is the step length in the propagation direction, $d = d_1 + d_2$ is the width of the superlattice unit cell, E_n is the subband energy, and k_z is the wave vector. Other quantities have conventional meanings. The periodic boundary conditions for Ψ are taken into account in constructing the matrix from the recursion relation. We investigated a noninteracting electron system and an interacting electron system (with electron-electron and electron-jellium interactions) in a uniformly doped and modulation-doped superlattice. It is well known that the effective mass (m^*) and the dielectric constant (ϵ_0) are the essential parameters of the model used in the present work, and thus care should be taken of their values and variations across the unit cell. Varying these parameters, we investigated their effect on the calculated quantities. We observed that our results are not affected in any essential manner when these parameters are within the commonly known values. The exchange potential expressed as a function of the local charge density is an ambiguous matter in the present method. However, we found that it is a very small fraction of the total potential. Recent developments in the effective-mass theory applied in the presence of an interface are extensively discussed in Ref. 9.

In Fig. 1 the potential profiles, $V(z)$, the lowest eight subbands, the Fermi level, and the charge densities are presented in the lower panels of (a), (b), and (c), corresponding to noninteracting, uniformly doped and modulation-doped systems, respectively. The corresponding wave functions $\Psi_n(k_z = 0, z)$ are illustrated in the upper panels. As shown in Fig. 1(a) the wave function of the state $n = 7$, which is just above the barrier in the noninteracting case (for a noninteracting free-electron gas) has large amplitude in the barrier region. As far as the energy location and the localization are concerned this state is reminiscent of the confined resonance states reported for a cell with different parameters.[4] We identify this state as CRS. This result is in agreement with the interpretation of state $n = 7$ as that derived from the lowest Γ valley of the alloy by Ninno, Wong, Gell, and Jaros.[10] It appears that the localization in the barrier region recedes as the subband energy rises above the barrier.

By comparing the potential profiles in Figs. 1(a) and 1(b) we see that in a uniformly doped superlattice a parabolic repulsive potential in the well region and an attractive potential in the barrier region are superimposed on the original potential. The repulsive potential arises because of the repulsion of the electrons occupying the confined states. The positively charged donor ions give rise to the attractive potential in the barrier region. In band-structure language these modifications in the potential barrier correspond to band bendings. The effect of the repulsive and attractive potential appears as shifts of the subbands. As seen in Fig. 1(b), the subbands below the potential minimum of the barrier are raised with respect to the subbands of the noninteracting electron system. In contrast to that the subbands above this minimum are lowered because of the additional binding provided by the superimposed attractive potential so that subbands 6 and 5 become closer to each other. Furthermore, the state $n = 6$ in Fig. 1(b) is localized in the $Ga_{1-x}Al_xAs$ barrier region. Interestingly, this state appears in the original barrier potential, V_0.

In Fig. 1(c), the modification of the square-well potential for a superlattice with modulated doping becomes even more pronounced because of the separation of positively and negatively charged particles. Similar to the case of uniform doping, the subbands are shifted because of the superimposed potential. Since the repulsive and attractive potentials here are much stronger than for uniform doping, the shifts in energies are accordingly larger, the Fermi level appears in a higher energy, and also the number of confined states is reduced as compared to the previous cases. In this case the state localized in the barrier appears $\sim$100 meV below the similar state seen in Fig. 1(a). This state ($n = 5$) has very large amplitude in the $Ga_{1-x}Al_xAs$ region and is $\sim$80 meV below the original potential barrier V_0. It is most interesting to note that the forms of the states localized in the $Ga_{1-x}Al_xAs$ region [state 6 in Fig. 1(b) and state 5 in Fig. 1(c)] are not significantly altered from that of the state 7 of Fig. 1(a), which was named as the confined resonance state. It appears that the effective barrier height is reduced as a result of the Coulombic interaction of excess charges, and thus the localized state of the noninteracting electron system [state 7 in Fig. 1(a)] shifts downward. On the basis of their similarities we identify these localized states [state 6 in Fig. 1(b) and state 5 in Fig. 1(c)] as the confined resonance states. It is seen that the stronger the attractive potential is the lower the CRS.

In conclusion, the Coulombic interactions among charged particles (ionized electrons and donor ions) are important and give rise to an appreciable amount of modification in the potential profile and band bending. This modification causes the subbands to shift and the Fermi level to rise. Moreover, the confined resonance states, which were previously reported to occur above the barrier,[4] form on the lower-lying states in the original barrier potential. This result has several important implications: First of all, the band bending due to the ionized donors and excess electrons in the conduction band reduces the effecitve barrier height, and thus it is an important factor for a realistic description of the confined resonance states. Therefore, this effect has to be included in the electronic band-structure or envelope-function models, wherefrom the quantum-well states are derived. Otherwise the absence of the Coulombic potential may lead to serious discrepancies. Another striking observation emerging from this study is that depending upon the level of doping and the size of the barrier, the position of the CRS with respect to the Fermi level undergoes a change affecting the transport properties and the mobility. Previously, low-temperature mobilities parallel to the layers in a modulation-doped superlattice were shown to decrease

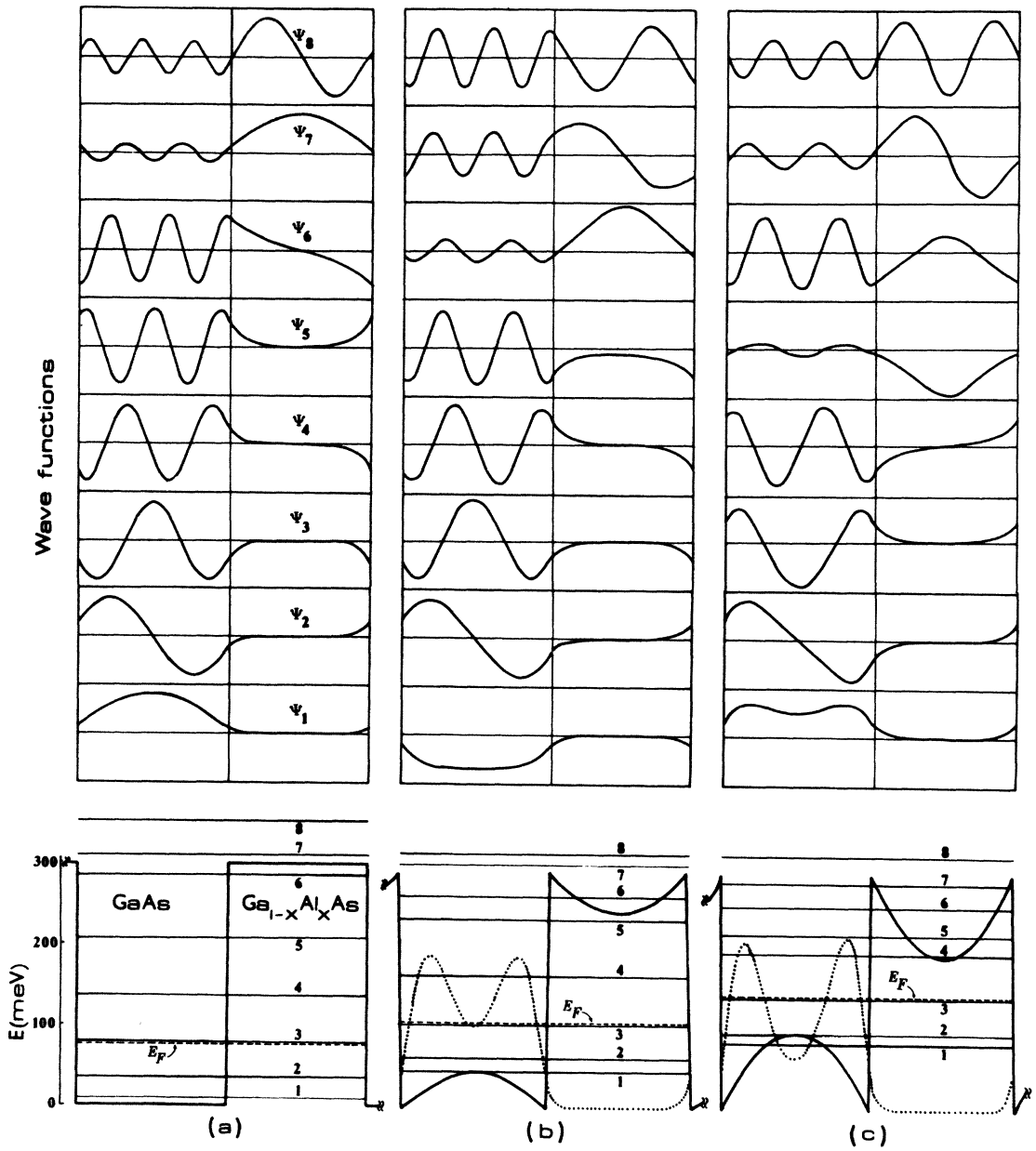

FIG. 1. Electronic states, potential, and charge density of the GaAs-$Ga_{1-x}Al_xAs$ superlattice calculated within the effective-mass theory. In lower panels: Thick lines, total one-dimensional potential, $V(z)$; the straight lines with numbers from 1 to 8 are subbands; dotted lines are total electronic charge density. In the upper panels the periodic part of the corresponding Bloch functions are illustrated. (a) Noninteracting electron gas, (b) uniform doping, (c) modulation doping with the Coulombic potential of electrons and ionized donors. The unit cell parameters used: The width of the well $d_1 = 221$ Å, the width of the barrier $d_2 = 218$ Å, the barrier height (or the discontinuity of the conduction band of GaAs and $Ga_{1-x}Al_xAs$) $V_0 = 300$ meV, the electron concentration in a unit area $N_S = 3.06 \times 10^{12}$ cm^{-2}. The effective mass of electrons $m^* = 0.068 m_0$ and the static dielectric constant $\epsilon_0 = 12.9$.

upon the inclusion of the band-binding effects.[8] In the present case the parameters of the supercell (V_0, d_1, d_2, and excess electron density) can be adjusted in such a manner that a CRS is lowered or may even dip into the Fermi level. Eventually, confined electrons can easily hop across the barrier, and thus the superlattice has higher conductivity along the z direction. This transition, which is reminiscent of a metal-insulator transition, should easily be observable experimentally.

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