RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 56, NUMBER 4 15 JULY 1997-II

Conduction-band mixing in T- and V-shaped quantum wires

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(Received 22 April 1997)

By means of a tight-binding approach, we have studied the influence of barrier states on the conduction band of the T- and V-shaped quantum wires. For AlAs/GaAs superlattices or pure AlAs barriers, X-related states induce strong modifications in the wire conduction band that cannot be accounted for by a simple effective-mass approximation. With respect to quantum wells, we show that the quasi-one-dimensional confinement of quantum wires enhances valley mixing and leads to a reduction in the energy of lower lying states. [S0163-1829(97)50628-X]

Quasi-one-dimensional (1D) confinement of electrons in semiconductor nanostructures [e.g., quantum wires (QWR's)] has been demonstrated in a variety of structures, based on direct etching, strain-induced quantum confinement, growth on vicinal substrates and so on. Recently, however, two approaches have attracted much attention. The first one consists in the growth of V-shaped quantum wire on a (100) GaAs substrate patterned with [01$\bar{1}$]-oriented V grooves.[1]

In this case, the GaAs wire is embedded in a AlAs/GaAs superlattice (SL) which constitutes the confining barrier for the electrons.[2,3] The second one is obtained from a cleaved-edge overgrowth technique which can produce very small (50 Å) GaAs T-shaped wires.[4,5] Here, the confining barriers consist of AlGaAs or pure AlAs layers.

Up to now the calculation of the band structure of these quantum wires has been limited by the huge dimension of the wire unit cell. The $\mathbf{k}\cdot\mathbf{p}$ method in the context of the envelope function approximation (EFA) is by far the most widely used.[3,6–8]

However, it has been shown that, despite the success in quantum wells, EFA breaks down for small quantum wires and quantum dots.[9–11] The restrictions of the EFA become very serious when indirect gap semiconductors are used in the wire (for example in Si wires) or in the barrier (AlAs or AlAs/GaAs superlattices). For these cases the use of *effective parameters*, e.g., effective barrier height, is highly questionable.

This paper presents a theoretical study of T- and V-shaped QWR's based on a tight-binding model which relaxes the restriction of EFA, maintaining at the same time the possibility to treat realistic structures. The latter characteristic, which implies calculations with more than 10^4 atoms in the unit cell, has been made feasible by recent developments in diagonalization algorithms.[12–15]

Empirical tight-binding calculations have already been performed for nm-size rectangular QWR's.[16] Reduction of the full tight-binding scheme to the effective bond orbital method (EBOM) has also been considered for V-shaped wires.[17] The latter approach is, however, similar to a $\mathbf{k}\cdot\mathbf{p}$ method, thus valid only for states near the zone center. Promising semiempirical pseudopotential methods[11] have been at present applied to ideal QWR geometries.

In the present study, we have used a sp^3s^* tight-binding including spin-orbit interaction.[18] The tight-binding parameters used in this calculation are adapted from Refs. 16 and 19, for $T=4$ K samples with a GaAs energy gap of 1.52 eV and an indirect AlAs gap of 2.24 eV. Effective masses are $m_\Gamma=0.0677$ for GaAs and $m_{X,l}=0.9$ for AlAs (l=longitudinal). The energy difference between Γ minimum of the first GaAs conduction band and the X minimum of the first AlAs conduction band is $\Delta_{\Gamma X}=160$ meV.[20] We should notice that experimental determinations of $\Delta_{\Gamma X}$ vary between 100 meV and 200 meV.[21–25] The number of atoms considered in the (large) unit cell of the wire is around 20 000 and in all the cases a check on the convergence of the results, as a function of the number of atoms, has been considered. Practically, all results are affected by a unit-cell truncation error smaller than 1 meV. Periodic boundary conditions are used at the boundary of the unit cell. The large Hamiltonian matrix H which results from such realistic dimensions of the unit cell, has been diagonalized by using a Lanczos algorithm without reorthogonalization. Following the folded spectrum method,[12,13] we do not directly diagonalize the Hamiltonian H but rather the matrix $A=(H-\lambda I)^2$ where λ (energy offset) defines an energy in the vicinity of which the eigenvalues are searched. With respect to the standard Lanczos algorithm, we have found that the lowest eigenstates of the associated tridiagonal matrix visit all the excited states of A before collapsing (Lanczos phenomena) on the lowest eigenvalue of A. This allows us to identify high-energy states during the Lanczos iteration. Eigenvectors (wave functions) can be obtained from the knowledge of the eigenvalues by using the inverse iteration technique.[15,26] The overall efficiency of the Lanczos/inverse iteration approach is very high and a typical band structure for realistic wire geometries can be carried out in a few hours of calculation on a workstation. Further details will be published elsewhere.[27]

T-shaped quantum wires are those of Ref. 5 and consist of an AlGaAs(500 Å)/GaAs(50 Å) SL grown along the [001] direction and a 50 Å quantum well in the [110] direction. The profile of the V-shaped quantum wire is that obtained from a TEM micrograph.[3,8,28] The confining barriers are created by embedding the GaAs V wire in a $(\mathrm{AlAs})_4/(\mathrm{GaAs})_8$ SL. The use of a SL with respect to the conventional AlGaAs barriers reduces the problems associated with the presence of

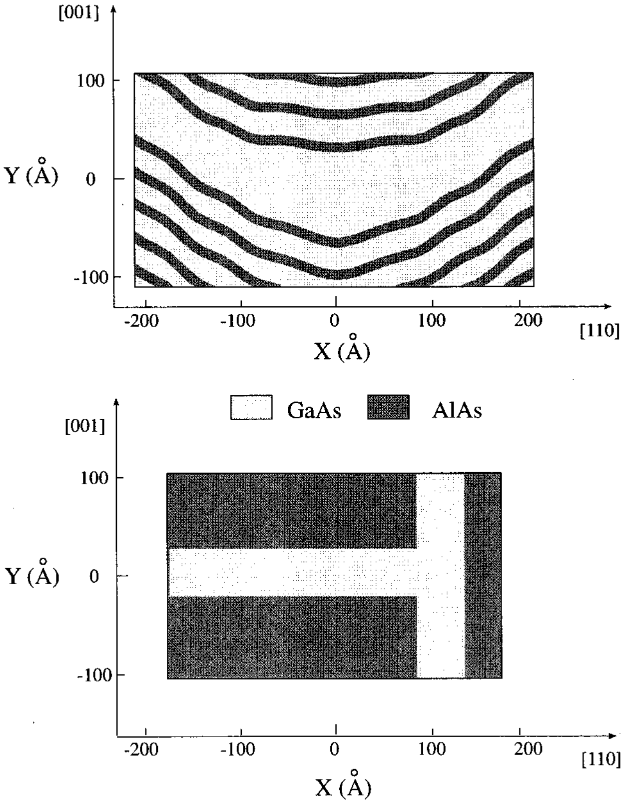

FIG. 1. Unit supercell used in the calculations for the V-shaped and T-shaped quantum wires.

alloy in the nanostructure. The unit cell used in our calculations for the V- and T-shaped QWR's is shown in Fig. 1.

The first conduction band of the the T-shaped wire for three different alloy compositions in the barrier is shown in Fig. 2. The calculation fully includes mixing between the Γ valley of the wire and the *X* valleys of the barrier. Experimentally,[29] indeed, it is well known that mixing induces a reduction of the barrier height with respect to the value obtained by simply considering the band discontinuity at the Γ point.

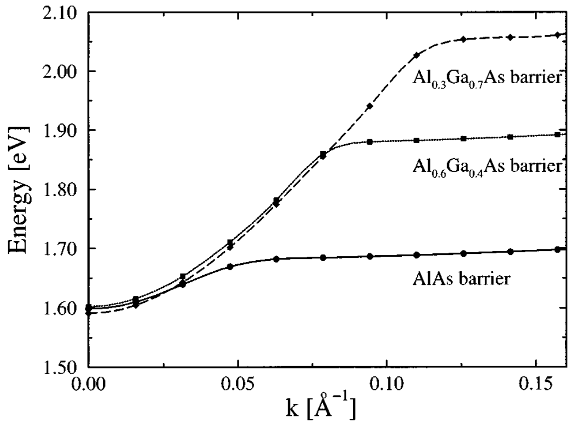

FIG. 2. First conduction band dispersion of the T-shaped quantum wire for three different alloy compositions of the barrier. The symbols represent the calculated points while the lines represent a cubic interpolation of these points. Spin (quasi) degenerate states are not shown.

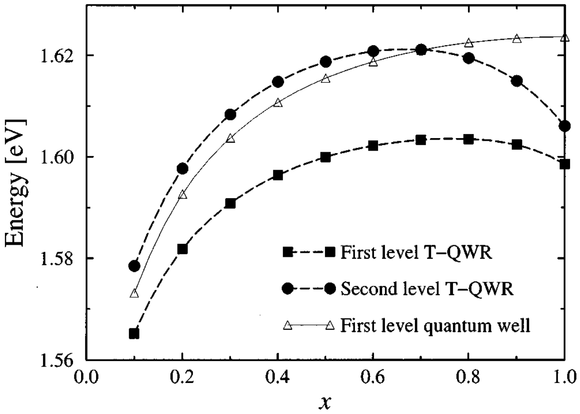

FIG. 3. Energy of the first two quantized levels in the conduction band for the T-shaped wire (symbols and dashed lines) as a function of Al barrier composition. The first quantized level for a 50 Å GaAs quantum well (thin continuous line) is shown for comparison.

Figure 2 clearly shows two distinct dispersion regions. The first one close to $k=0$ is related to the GaAs Γ valley of the wire. The associated electron wave function is confined to the wire and the calculated band dispersion is similar to that obtained in the one-band effective-mass approximation. However, the electron effective mass in this region increases from $m^*=0.075$ for QWR's with $Al_{0.3}Ga_{0.7}As$ barriers to $m^*=0.088$ for QWR's with AlAs barriers.

The second region at larger *k*'s displays a flat band dispersion with high electron mass. Since the energy onset of this region varies with Al barrier content, those states are clearly related to the *X* valley of the AlGaAs barrier. The corresponding wave function of these states is mainly extended in the barrier. Γ related states of the wire can still be found for energies higher then the *X* minimum, however, the strong coupling between *X* and Γ states will reduce their lifetime.[20,30]

The energy of the $k=0$ state of the first two conduction subbands as a function of the barrier alloy concentration is shown in Fig. 3. By increasing the Al content one should expect a continuous enhancement of confinement due to the higher and higher barrier. However, due the Γ-*X* mixing, the quantization energy reaches a maximum around $x=0.7$ and decreases for higher Al contents. Such behavior would not be detected by using an effective-mass approximation where, by increasing the alloy concentration and consequently the barrier height, the quantization energy would tend to saturate to the value obtained from the infinite barrier model. As expected, Γ-*X* mixing increases for higher energy states. Indeed, wires with AlAs barriers show a reduction of 15 meV for the second level position and only 5 meV for the first one with respect to the ones with $Al_{0.7}Ga_{0.3}As$ barriers. We also notice that the energy difference between first and second level is higher for an Al concentration between $x=0.6$ and $x=0.7$ and it is strongly reduced for AlAs barriers. Such observation has important practical implications, as it defines an optimal level separation, a property which controls, e.g., the characteristics (linewidth, threshold, linearity) of QWR lasers. Thus, the use of $Al_xGa_{1-x}As$ barriers for T-shaped wires with x around 0.7 leads to high quantization energy,

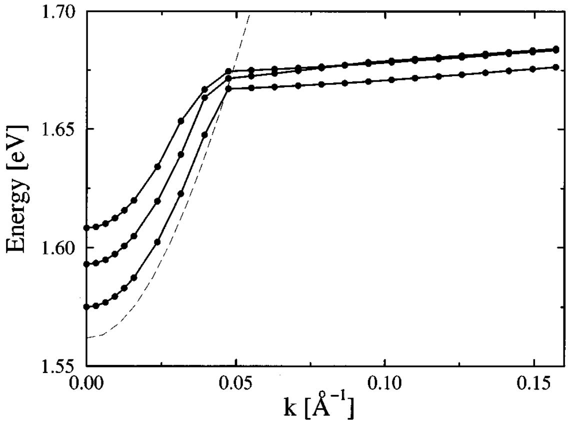

FIG. 4. Conduction band dispersion for the first three levels of the V-shaped quantum wires. The symbols represent the calculated points while the continuous lines represent an interpolation of these points. The dashed line represents the first conduction band for a V-shaped wire with AlGaAs barrier and a barrier high of 0.15 eV. Spin (quasi) degenerate states are not shown.

reduces the penalty due to X states at too low energies and maximizes the energy separation between first and higher levels. The quantization energy of the ground level can be further increased by reducing the wire dimension. However, in this case, the wire may suffer a $\Gamma \rightarrow X$ transition and become type-II, as already observed in Ref. 11.

For sake of comparison, Fig. 3 also shows the position of the ground level for a 50 Å GaAs/AlGaAs quantum well as a function of the barrier Al concentration. No reduction of quantization energy is observed at high Al concentration. Such behavior is independent on well width. We can therefore conclude that, *the strength of* Γ-X *mixing increases with the reduction of dimensionality*. This can be explained by considering that valley mixing results from breaking of the translational symmetry in the presence of heterojunctions.

The three lowest subband dispersions (along the wire-free direction) of a V-shaped wire are shown in Fig. 4. As seen for the T structure, the dispersion consists of a low-energy region related to the Γ valley of GaAs followed by a flat region related to the barrier states. The confinement energies at $k=0$ for the first three subbands are 55, 73, and 88 meV, respectively, which are lower with respect to those of the T wire with AlAs barriers. The flat portion of the dispersion also presents distinct levels, a consequence of the quantization of superlattices states. In T-shaped wire, barrier states are not quantized.

For comparison, Fig. 4 shows the first subband dispersion for a V wire obtained with AlGaAs barriers assuming a band discontinuity ΔE_c of 0.15 eV. This is the value recently used as an effective barrier height to mimic the confinement of the AlAs/GaAs superlattice.[3,31] For the V wire with AlGaAs barrier we obtain a confinement energy at $k=0.0$ for the first and second subband of 42 meV and 55 meV, respectively, very close to those calculated in Refs. 3 and 31 (43.31 and 57.28 meV, respectively). However, these confinement energies underestimate those obtained with the real superlattice barrier. Indeed, the energy difference between the two situations is equal to 13 meV for the first subband and increases up to 18 meV for the second. A better agreement is found when the barrier Al content is increased at $x=0.5$.

In conclusion, a tight-binding analysis of QWR has shown that band mixing between wire Γ states and barrier X states can drastically change the electronic properties of the conduction band in T- and V-shaped structures. Γ-X mixing is enhanced in quantum wires, where the translational symmetry is broken in two dimensions, with respect to systems where the symmetry is broken in just one dimension (e.g., quantum well, superlattices). Such mixing cannot be accounted for within the effective-mass approximation since the band discontinuity is not simply given by the profile of the Γ point energy. As a consequence, all effective-mass results related to the barrier height can be affected by the restriction of the effective-mass model. Γ-X mixing can reduce, for high alloy concentration, the quantization energy. We have found for the T wires an optimal Al content for the barrier ($x=0.7$) which maximizes the quantization energy and the energy separation between ground level and higher excited states.

We acknowledge TRACS support.

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