Confined electron states in GaAs-$Ga_{1-x}Al_xAs$ quantum wires

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We present a quantitative theory of the electronic levels in GaAs-$Ga_{1-x}Al_xAs$ ⟨001⟩ quantum wires ($x \leq 0.35$). For the ground state of thick wires (cross-section area $\gtrsim 100\times100$ Å^2) our results support the infinite-well approximation in which the two quantization coordinates are decoupled. However, the excited states, and all confined states in thin wires ($\lesssim 70\times70$ Å^2), are affected by additional reflections which can be identified from tables of the momentum wave-function coefficients presented in this study.

Recently, it has become possible to fabricate quantum-wire structures (QWS's) of submicron dimensions.[1] Apart from the obvious academic interest in such a new structure, there are a number of practical applications. They stem from the one-dimensional character of the confining potential which may, for example, give rise to higher electron mobilities and deeper exciton binding energies.[2,3] The electronic properties of QWS's have been modeled in the framework of approximate schemes[2,3] in which the coordinates perpendicular to the wire axis are assumed to be independent. The confined bound states are then found by solving the effective-mass Schrödinger equation for a particle-in-a-box problem with infinite barriers. The energy levels can be characterized by quantum numbers (n_x,n_y) derived from the uncoupled one-dimensional square-well problem. However, in a realistic model of the QWS, the potential representing the individual layers is finite and motion in the two directions is not separable. This imposes severe difficulties in defining basis functions for the effective-mass equation, and we have not found a satisfactory solution in the literature. In this study, we report the first full-scale calculation of the effect of confinement in GaAs-$Ga_{1-x}Al_xAs$ ⟨001⟩ QWS's. We present energy levels and wave functions for several systems and show that at least in some of the confined levels the coupling between the two quantization directions is significant and leads to different energy levels.

In our calculations a GaAs-$Ga_{1-x}Al_xAs$ QWS is realized by embedding ultrathin wires of GaAs in a confining barrier material such as $Ga_{1-x}Al_xAs$. The two-dimensional potential well at the interfaces between the two materials confines electrons to move along the axis of the wire, which forms a quasi-one-dimensional electron gas in the ⟨001⟩ direction. Our method of calculation is a natural extension of the approach used to model conventional superlattices.[4,5] It has been demonstrated that our technique can yield energy levels and transition energies in conventional GaAs multiple-quantum-well structures with a meV accuracy and correctly accounts for oscillator strengths of allowed as well as "forbidden" transitions.[6] We expand the wave function ψ of a GaAs-$Ga_{1-x}Al_xAs$ QWS in terms of the complete set of Bloch functions $\phi_{n,\mathbf{k}}$ satisfying the Schrödinger equation $(H_0-E)\phi_{n,\mathbf{k}}=0$ where n is the band index, $\mathbf{k}$ is the bulk reduced wave vector, and H_0 is an infinite-crystal Hamiltonian for GaAs. The QWS Hamiltonian is $H=H_0+V$, where V is the difference between pseudopotentials in the two materials. The Schrödinger equation to be solved is then

$$(H_0+V-E)\sum_{n,\mathbf{k}} A_{n,\mathbf{k}}\phi_{n,\mathbf{k}}=0 \ . \tag{1}$$

A rectangular block of GaAs-$Ga_{1-x}Al_xAs$ has been chosen to be the unit cell. Its dimensions are 30 lattice constants (we have used the same lattice constant, 5.653 Å, for both materials) along both the ⟨100⟩ and ⟨010⟩ directions and one lattice constant along the ⟨001⟩ direction which is the quantum-wire axis. Different sizes of quantum wire can be studied using the same unit cell but with different proportions of GaAs and $Ga_{1-x}Al_xAs$ inside it. Considering a cross section of the unit cell in the (001) plane, GaAs occupies a square in the middle of the unit cell. This structure will be repeated in both the ⟨100⟩ and ⟨010⟩ directions with a periodicity of 30 lattice constants and in the ⟨001⟩ direction with same periodicity as the bulk material. Hence in the system described above, V in Eq. (1) will be a periodic potential and the Bloch functions $\phi_{n,\mathbf{k}}$ that contribute to ψ will be unambiguously determined. Therefore,

$$V=\sum_j [V_j(Ga_{1-x}Al_xAs)-V_j(GaAs)] \ , \tag{2}$$

where j runs through all sites of $Ga_{1-x}Al_xAs$ in the unit cell. The sampling of Bloch functions is taken over one plane in the bulk face-centered-cubic Brillouin zone. For instance, at the center of the Brillouin zone (Γ) of the QWS a two-dimensional grid of sampling points separated by a distance of $2\pi/30a$ (where a is the lattice constant) is taken in the octagonal (001) plane. After determining the periodic potential V and set of basis functions $\phi_{n,\mathbf{k}}$, we can multiply Eq. (1) from the left by $\phi^*_{n',\mathbf{k}'}$ and integrate over the volume to recover an eigenvalue equation

$$A_{n',\mathbf{k}'}(E_{n',\mathbf{k}'}-E)+\sum_{n,\mathbf{k}} A_{n,\mathbf{k}}\langle\phi_{n',\mathbf{k}'}\mid V\mid\phi_{n,\mathbf{k}}\rangle=0 \ . \tag{3}$$

This equation is familiar from our earlier work on impurities and dislocations[7,8] and is solved by direct diagonalization.

It should be noted that in the above formulation we

have employed the virtual-crystal approximation to model the alloy. We have also adjusted both GaAs and $Ga_{1-x}Al_xAs$ band structures and their relative alignment in a manner which we have published in detail elsewhere.[5,9] The relative positions of principal symmetry points in both band structures and the band offset are in good agreement with experiment. To indicate the height of the confining barrier in the two-dimensional square well, the positions of the bulk band minima are included in Table I. Since the aim of this report is to understand the confinement process in a one-dimensional system, we have limited our attention to the conduction states only. We begin with a calculation of the electronic structure of GaAs-$Ga_{0.7}Al_{0.3}As$ QWS's where the size of the GaAs quantum well is 102×102 Å^2. The energy spectrum near the conduction-band edge, obtained in our calculation at the center of the QWS Brillouin zone (i.e., at Γ) is shown in Table I. All C_1 to C_8 are confined states for which the electron charge densities are found mainly in the GaAs well. State C_R is a resonance lying above the barrier as seen in conventional superlattices.[4] State X_1 is the X-related confined state. Since X_c(GaAs) is above $X_c(Ga_{0.7}Al_{0.3}As)$, state X_1 is localized in the $Ga_{0.7}Al_{0.3}As$ barrier. The effective mass of the X valley is large and, as expected, there is a series of closely spaced confined states above state X_1. These states are not listed in Table I. The electron charge densities associated with the first six states (C_1–C_6) and states C_R and X_1 are plotted in Fig. 1. The average charge densities for the low-lying confined states are the same as those expected from the simple model (i.e., the product of two cosine functions). It is worth mentioning that states C_2 and C_3 are degenerate and the expected form of their charge densities can be recovered by taking a linear combination of their wave functions. Even the energy of the ground state agrees with the assumption that there is no coupling between the two transverse directions perpendicular to the quantum-wire axis (i.e., an infinite well). In a calculation for a conventional GaAs-$Ga_{0.7}Al_{0.3}As$ superlattice system with a 102-Å GaAs well and with the same periodicity as in the QWS calculation, we find that the ground state is 28 meV above the bottom of the GaAs conduction-band edge. Since we have taken a two-dimensional GaAs well, the quantizations in the interface plane are the same in both directions and the sum of their contribution is 56 meV. In the QWS calculation the ground-state energy obtained is also 56 meV. However, this is not the case in small QWS's. Consider three different QWS systems. Case A corresponds to the above calculation with a 102×102-Å^2 GaAs well (barrier thickness 68 Å), while cases B and C correspond to 68×68-Å^2 and 34×34-Å^2 wells, respectively. The ground-state energies of these QWS's are 56 meV, 101 meV, and 215 meV, respectively. For cases B and C the discrepancies between our calculation and the value expected from the simple model are 3 meV and 25 meV, respectively. In fact, our calculations predict several excited states which are lower than the sum of the two quantization energies. There are two reasons for these discrepancies. Firstly, the energy of a confined state in a QWS obeys the sum rule only in an infinite quantum well. This can be realized from the fact that there always exists at least one bound state in a two-dimensional square well. For a finite two-dimensional well, it is possible to find a bound state in which the sum

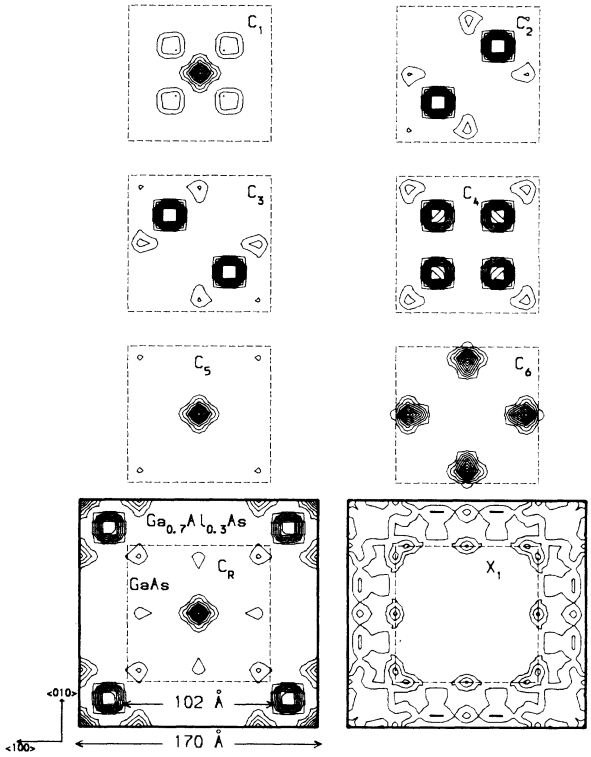

FIG. 1. Electron charge densities of some of the confined states reported in Table I. Since states C_1–C_6 are all confined in GaAs, only the quantum-wire portions (i.e., GaAs wells) in the unit cell are shown for these states. State C_R lies above the barrier and is localized in the barrier material. State X_1 is the lowest state derived from the secondary X minima. Both C_R and X_1 have analogous properties to those obtained for such states in conventional superlattices (see Refs. 4 and 5).

TABLE I. A table showing the energy levels calculated for GaAs-$Ga_{0.7}Al_{0.3}As$ QWS's at the center of the Brillouin zone (i.e., at Γ). The energies are measured in meV from the conduction-band edge of bulk GaAs, i.e., Γ(GaAs). The quantum-wire thickness is 102×102 Å^2. The barrier thickness is 68 Å. The bulk conduction-band minima $\Gamma(Ga_{0.7}Al_{0.3}As)$, $X(Ga_{0.7}Al_{0.3}As)$, and X(GaAs) are 285 meV, 394 meV, and 489 meV above Γ(GaAs), respectively.

State	Energy (meV)
C_1	56
C_2	134
C_3	134
C_4	204
C_5	234
C_6	239
C_7	294
C_8	294
C_R	328
X_1	396

TABLE II. A table showing the moduli squared of the leading coefficients $A_{n,\mathbf{k}}$ in Eq. (1) for the ground state in three cases A, B, and C for both $\mathbf{k}_{\langle 100\rangle}$ and $\mathbf{k}_{\langle 010\rangle} \geq 0$. The thickness of the quantum wire in cases A, B, and C are 102×102 Å^2, 68×68 Å^2, and 34×34 Å^2, respectively. Wave vector $\mathbf{k}$ is in units of $2\pi/30a$, where a is the lattice constant. Only coefficients for the conduction band are shown. The normalization is chosen such that $\sum_{n,\mathbf{k}} |A_{n,\mathbf{k}}|^2 = 1$.

	$\mathbf{k}_{\langle 100\rangle}$	$\mathbf{k}_{\langle 010\rangle}$	$\mathbf{k}_{\langle 001\rangle}$	A	B	C
At Γ	0.0	0.0	0.0	0.443	0.291	0.316
Along $\langle 100\rangle$	1.0	0.0	0.0	0.109	0.112	0.093
	2.0	0.0	0.0	0.000	0.008	0.012
Along $\langle 010\rangle$	0.0	1.0	0.0	0.109	0.112	0.093
	0.0	2.0	0.0	0.000	0.008	0.012
Off axial	1.0	1.0	0.0	0.029	0.048	0.041
	1.0	2.0	0.0	0.000	0.004	0.008
	2.0	1.0	0.0	0.000	0.004	0.008
	2.0	2.0	0.0	0.000	0.000	0.003

of its one-dimensional quantization energies is larger than the strength of the potential. In case A it is valid to say that the quantum well is infinite as far as the ground state is concerned. It is not true for cases B and C. Secondly, interactions between the two quantization directions exist and contribute to the confinement of electrons in the two-dimensional quantum well.

To trace the evidence concerning the coupling between the two quantization directions, we look at the coefficients $A_{n,\mathbf{k}}$ in the expansion of the wave function ψ. In Table II, we show the moduli squared of the leading $A_{n,\mathbf{k}}$ coefficients for the ground states in the above three calculations. Only the lowest conduction-band contribution is tabulated as this is the dominant term in the expansion. Also, since potential V in Eq. (2) is invariant under reflections along the $\langle 100\rangle$ and $\langle 010\rangle$ directions, we list only coefficients which correspond to $\mathbf{k}_{\langle 100\rangle}, \mathbf{k}_{\langle 010\rangle} \geq 0$. From Table I, we can see the quantum-wire ground state in case A is derived mainly from contributions along the two quantization directions $\langle 100\rangle$ and $\langle 010\rangle$. There are rarely any terms in the expansion from the off-axial Bloch functions (i.e., Bloch functions corresponding to both $\mathbf{k}_{\langle 100\rangle}$ and $\mathbf{k}_{\langle 010\rangle}$ not equal to zero). When the off-axial terms become important in cases B and C, we find a coupling between the two quantization directions affecting the energy levels. Physically, these off-axial terms could correspond to standing waves formed by multiple reflections other than those between opposite (001) interfaces in the two-dimensional quantum well.

More evidence to show the existence of coupling between the two quantization directions can be seen from the confined excited states. Let us study C_2, C_3, and C_4 in Table I again. We have already mentioned above that the ground-state energy is 28 meV in a superlattice with a 102 Å GaAs well. Furthermore, we know that the first excited state is of energy 110 meV. Therefore, we would expect the energies of C_2 and C_3 to be 138 meV and C_4 to be 220 meV. We recover in our calculation the energies of C_2 and C_3 to be 134 meV and C_4 to be 204 meV, respectively. As far as higher states are concerned, they no longer see an infinite well. A similar evidence about the $A_{n,\mathbf{k}}$ coefficients as described above exists to explain these differences. In Table III we can see the significance of off-axial terms in the expansion of the wave function of state C_2 to C_4. The importance of the additional reflections is also supported by the properties of states C_4, C_5, and C_6. In the expansion of state C_4, there is hardly any contributions at all from k points along the $\langle 100\rangle$ and

TABLE III. A table showing the moduli squared of the leading coefficients $A_{n,\mathbf{k}}$ in Eq. (1) for three excited states in Table I for both $\mathbf{k}_{\langle 100\rangle}$ and $\mathbf{k}_{\langle 010\rangle} \geq 0$. $\mathbf{k}$ is in units of $2\pi/30a$, where a is the lattice constant. Also, only coefficients for the conduction band are shown and the same normalization as in Table II is chosen.

	$\mathbf{k}_{\langle 100\rangle}$	$\mathbf{k}_{\langle 010\rangle}$	$\mathbf{k}_{\langle 001\rangle}$	State C_2	State C_3	State C_4
At Γ	0.0	0.0	0.0	0.000	0.000	0.000
Along $\langle 100\rangle$	1.0	0.0	0.0	0.134	0.159	0.000
	2.0	0.0	0.0	0.018	0.021	0.000
Along $\langle 010\rangle$	0.0	1.0	0.0	0.159	0.134	0.000
	0.0	2.0	0.0	0.021	0.018	0.000
Off axial	1.0	1.0	0.0	0.142	0.142	0.193
	1.0	2.0	0.0	0.006	0.006	0.025
	2.0	1.0	0.0	0.005	0.007	0.025
	2.0	2.0	0.0	0.000	0.000	0.006

⟨010⟩ directions. The formation of state C_4 can only be explained in terms of interactions different from those in the intuitive picture. States C_5 and C_6 behave differently from the effective-mass theory, and they are split by 5 meV. For completeness, we might add that the variation of the energies of states C_1 to C_3 of case A with different aluminium concentration in the alloy material of the QWS follow the trend expected on intuitive grounds and offer no surprising results.

In summary, we have reported the first quantitative study of the electronic structure of GaAs-$Ga_{1-x}Al_xAs$ quantum-wire structures. We have demonstrated the limits of applicability of the simple infinite-well model and conclude that in thick quantum wires ($\gtrsim 100\times 100$ Å^2) this model is valid for the lowest-lying state. For thinner quantum wires, the coupling effects are more pronounced and affect all levels. The additional reflections responsible for the change in energy levels can be identified from the momentum wave-function coefficients presented in this paper.

[1]P. M. Petroff, A. C. Gossard, R. A. Logan, and W. Wiegmann, Appl. Phys. Lett. **41**, 635 (1982).
[2]H. Sakaki, Jpn. J. Appl. Phys. **19**, L735 (1980).
[3]V. K. Arora, Phys. Rev. B **23**, 5611 (1981).
[4]M. Jaros and K. B. Wong, J. Phys. C **17**, L765 (1984).
[5]K. B. Wong, M. Jaros, M. A. Gell, and D. Ninno, J. Phys. C **19**, 53 (1986).
[6]D. Ninno, M. A. Gell, and M. Jaros, J. Phys. C **19**, 3845 (1986).
[7]M. Jaros, *Deep Levels in Semiconductors* (Hilger, London, 1982).
[8]M. J. Kirton and P. W. Banks, J. Phys. C **17**, 2475 (1984).
[9]M. A. Gell, D. Ninno, M. Jaros, and D. C. Herbert, Phys. Rev. B **34**, 2416 (1986).