ENERGY LEVELS IN QUASI UNI-DIMENSIONAL SEMICONDUCTOR HETEROSTRUCTURES

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We report calculations of valence levels in quasi one-dimensional semiconductor heterostructures. Subband mixing is considered and the subband dispersions along the wire-axis direction are calculated for GaAs/Ga(Al)As quantum wires.

In the last years some progress has been achieved in reducing the sizes of semiconductor heterostructures. Quasi uni- dimensional semiconductors[1-3] have been obtained via sophisticated growth, etching and cutting techniques. In ideal unidimensional structures the carrier motion along two directions (z and x) is bound while it is free along the third one (y). The carrier mobility has been estimated to be enhanced over the bulk and two-dimensional values in the Electric Quantum Limit[4] due to the reduction of the available phase space for the scattering events. On the other hand, it is not clear that the assumption underlying the predicted mobility enhancement, which is that the carrier wavefunctions are spatially extended, can be reconcilied with the general statement that all states are spatially localized in quasi uni-dimensional materials. Recently, some new types of quasi-unidimensional semiconductor structures have been theoretically proposed. Chang et al[5] studied a non-rigid quasi uni-dimensional structure which is obtained by converting one side of the potential barrier of an asymmetric quantum well into a periodically indented potential. Laux and Stern[6] performed a self-consistent calculation for a narrow gate $Si-SiO_2$ MOSFET, and Lai and Das Sarma[7] proposed analytical variational calculations in narrow inversion MOSFET layers. The present authors[8] have considered decoupled calculations for the study of one-side, spike-doped GaAs/Ga(Al)As semiconductor wires. All these calculations involved conduction subband levels. To the best of our knowlegde, no valence levels were studied until now. We propose here an approximate method for computing these valence levels and their subband dispersions along the direction of the wire-axis.

We use the effective-mass approximation. The valence bands are described by the Luttinger[9] Hamiltonian where we only retain the Γ_8 bands. The spin-orbit splitting is taken as infinite. The Γ_6 conduction band and the remote bands are considered to second-order in k and are described by the Luttinger parameters. The Schrödinger equation to be solved is

$$[\underline{H}_8 + V(x,z)\underline{1}]\,\vec{\psi}_k = \varepsilon\,\vec{\psi}_k \qquad (1)$$

where $\underline{H}_8$ is the 4x4 Luttinger Hamiltonian (see eq. 32 of ref. 10), $\underline{1}$ is a 4x4 unit matrix and $\vec{\psi}_k$ is a 4x1 column vector. We consider rectangular semiconductor wires and neglect band warping as well as eventual mismatches between Luttinger parameters of the host materials. The potential energy V(x,z) can be splitted in the form (see fig. 1)

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Fig. 1- Splitting of the (x,y) dependent potential energy V(x,y) of a rectangular quantum wire in terms of a z dependent term $V_b(z)$ and a correcting term w(x,z). The dashed areas correspond to zero potential regions.

$$V(x,z) = V_b\, Y(z^2 - L_z^2/4)\, Y(x^2 - L_x^2/4) = V_b(z) + w(x,z) \qquad (2)$$

where

$$V_b(z) = V_b\, Y(z^2 - L^2/4) \qquad (3.a)$$

and

$$w(x,z) = V_b\, Y(x^2 - L_x^2/4)\, Y(L_z^2/4 - z^2) \qquad (3.b)$$

Y(x) is the step function (i.e., equal to 1 for $x > 0$ and 0 for $x < 0$). V_b is the valence barrier height and L_x and L_z are respectively the x and z quantum wire thicknesses. We solve eq. 1 using an approximate scheme which consists of writing

$$\vec{\psi}_k = \begin{bmatrix} \sum_{i,m} \alpha_{im}^{+}(k_y)\, \chi_i(z)\, \xi_{im}(x) \\ \sum_{j,n} \beta_{jn}^{-}(k_y)\, \varphi_j(z)\, \zeta_{jn}(x) \\ \sum_{j,n} \beta_{jn}^{+}(k_y)\, \varphi_j(z)\, \zeta_{jn}(x) \\ \sum_{i,m} \alpha_{im}^{-}(k_y)\, \chi_i(z)\, \xi_{im}(x) \end{bmatrix} \times 1/\sqrt{L_y}\, \exp(ik_y y) \qquad (4)$$

where $\chi_i(z)$ ($\varphi_j(z)$) are the heavy (light) hole eigenfunctions at $k_y = 0$ for the z decoupled motion confined by the potential $V_b(z)$. $\xi_{im}(x)$ and ($\zeta_{jn}(x)$) are the solutions of the zeroth order diagonal part of eq. 1 for the x motion at $k_y = 0$[7]. For the heavy-hole, for example, the latter functions are obtained by solving the equation

$$[a_+ + \int \chi_i^2(z)\, w(x,z)\, dz]\, \xi_{im}(x) = E_{im}\, \xi_{im}(x) \qquad (5)$$

where a_+ is the heavy-hole diagonal part in eq. 1. This zeroth order approximation is all the more valid when the size quantization along x is smaller than that along z. We should remark that the E_{im}'s are not the zeroth order solutions of the x motion at $k_y = 0$ since there are also non-zero x-dependent off-diagonal terms at $k_y = 0$ in $\underline{H}_8$. The true confinement energies for the semiconductor quantum wire are obtained, for any value of k_y, by projecting the Hamiltonian $\underline{H}_T = \underline{H}_8 + V(x,z)\underline{1}$ on the basis given in eq. 4. The eigenvalues are obtained by numerical diagonalization.

In fig. 2 we show the subband dispersion along k_y for three rectangular quantum wires of GaAs cladded by $Ga_{0.8}Al_{0.2}As$ (full lines) whose dimensions are $L_z = 50$ Å, and a) $L_x = 100$ Å, b) $L_x = 150$ Å and c) $L_x = 200$ Å. The dashed lines show the subband dispersion along a direction parallel to the layers (x,y) of such a $GaAs/Ga_{0.8}Al_{0.2}As$ quantum well ($L_z = 50$ Å). The Luttinger parameters used are $\gamma_1 = 6.85$, $\bar{\gamma} = (2\gamma_2 + 3\gamma_3)/5 = 2.58$. The valence barrier height is 100 meV. We observe that, for a quantum wire, we cannot label the eigenfunctions at $k_y = 0$ as heavy- and light-hole subbands. The off-diagonal terms strongly mix these subbands and m_J is no longer a good quantum number. This subband mixing increases with k_y. However, in some cases, the eigenfunctions are not much changed with respect to the diagonal approximation. For example, in fig. 2.a the levels labelled 1(2) have about 94% (90%) of the first x,z heavy(light)-hole character. In the same way, the 4th level has 61% of the first diagonal x-quantization of the second z-heavy-hole subband. If we inspect the subband dispersions of these three levels we can see that, for small values of k_y, they more or less reproduce the quantum well in-plane dispersion (dashed lines). With increasing L_x we have more levels quantized in the x-direction, enlarging the family of basis levels attached to each z-quantized level. The subband mixing is strong since the levels at $k_y = 0$ are close in energy. As expected, the off-diagonal coupling terms replace the crossings by anticrossings in the subband dispersion, a behavior already observed in the in-plane quantum well dispersions[10,11]. In fig. 3 we have plotted the k_y subband dispersion of a $GaAs/Ga_{0.8}Al_{0.2}As$ quantum wire with $L_z = 100$ Å and $L_x = 200$ Å thicknesses. The large number of subbands created by the x,z quantization and the small value of their energy separation lead to a strong coupling amongst the subbands. In reality the x-quantization has almost fade away.

In conclusion, we have presented the first calculations of the valence subband dispersion relations GaAs-Ga(Al)As

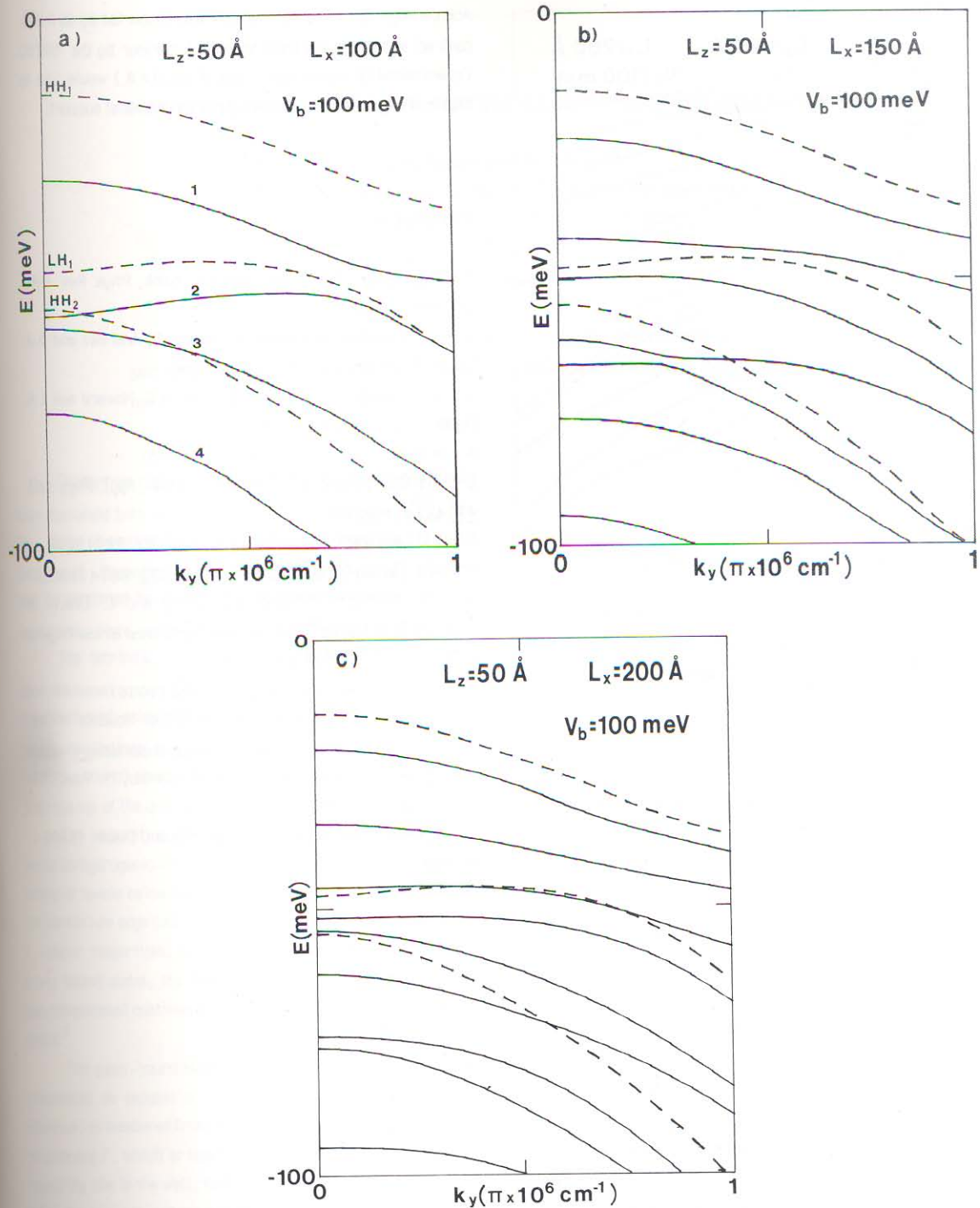

Fig. 2- Calculated valence subband dispersions along the wire axis of GaAs-$Ga_{0.8}Al_{0.2}As$ quantum wires (solid lines). L_z = 50 Å. L_x = 100 Å, 150 Å, 200 Å in figs. 2.a, 2.b, 2.c respectively. The dashed lines represent the valence subband dispersions of a 50 Å thick GaAs-$Ga_{0.8}Al_{0.2}As$ quantum well. The zero of energy corresponds to the GaAs valence band edge.

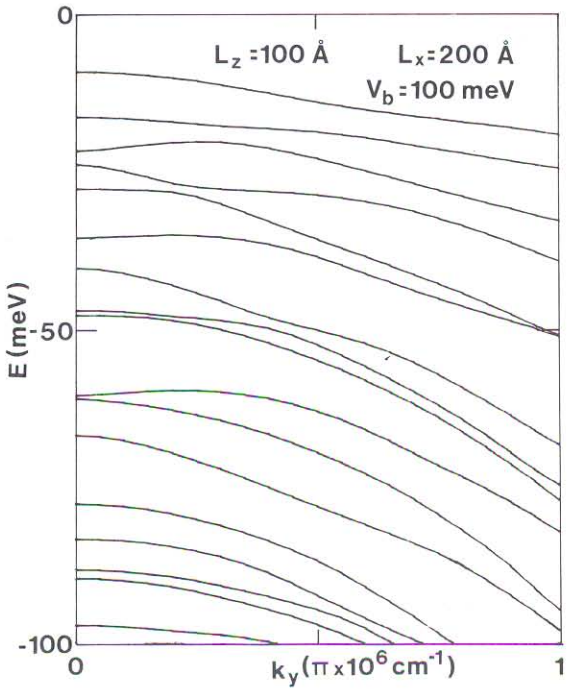

Fig. 3- Calculated valence subband dispersions along the wire axis of a GaAs-$Ga_{0.8}Al_{0.2}As$ quantum wire. L_z = 100 Å. L_x = 200 Å. The zero of energy corresponds to the GaAs valence band edge.

quantum wires along the wire axis. Strong subband couplings are actually present, even for the k_y = 0 levels. This subband mixing should be considered in the study of exciton and acceptor structures.

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