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Valence-band Energies of GaAs/AlGaAs and InGaAs/InP V-groove $[1\bar{1}0]$ Quantum Wires

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ABSTRACT

Comparison between the Burt-Foreman and Luttinger-Kohn valence-band Hamiltonians have been performed for realistic V-groove GaAs/AlGaAs and InGaAs/InP quantum wires. Significant differences in band structure is only found for InGaAs/InP quantum wires.

Keywords: quantum wires, V-groove, $k \cdot p$ theory, valence band, band structure

1 INTRODUCTION

High quality V-groove GaAs/AlGaAs quantum wires (QWR's) of nanometer cross-section have been grown by low pressure organometallic chemical vapor deposition techniques [1]. The structural parameters and quality were initially ascertained using conventional and high resolution transmission electron microscopy, and by low-temperature cathodoluminescence [1]. Subsequently, low temperature polarized photoluminescence and polarized photoluminescence excitation (PLE) experiments were carried out and, together with a $k \cdot p$ calculation, it was deduced that the optical transitions involved one-dimensional excitons and that a strong suppression of the band-edge absorption occured [2], [3].

The calculation was crucial in labeling the nature of the structures in the optical spectra. In the original papers [2], [3], a one-band parabolic effective-mass equation was used for the conduction states and a four-band Luttinger-Kohn Hamiltonian was used for the valence states. Excitonic corrections were *ad hoc* accounted for by rigidly redshifting the theoretical single-particle transition energies by 10-20 meV for each structure investigated. Excellent agreement was thus obtained between theory and low-incident-angle linearly polarized PLE spectra (on planarized structures in order to minimize surface grating effects) for the 2.5 nm structure (the dimension being the thickness of the crescent region of the QWR), but not so for the other two structures (5 nm and 1.5 nm QWR's). We note that Stier and Bimberg had carried out an eight-band calculation [4] but concentrated on piezoelectric effects.

The goal of this work is to investigate whether the discrepancy between the theory and experiment in [3] is band-structure related. Specifically, we address the issue of whether the Luttinger-Kohn (LK) Hamiltonian is appropriate for this QWR structure. The theoretically correct Hamiltonian has been shown to be the so-called Burt-Foreman (BF) one [5], [6]. Foreman had shown that the two can give very different heavy hole (hh) effective masses for InGaAs/GaAs (001) quantum wells (QW's). Meney *et al.* [7] had also shown that the four-band BF Hamiltonian gives different band structures compared to the LK one for 10 nm GaAs/AlAs (001) QW's, especially for intermediate wave vectors, with energy differences of up to 10 meV. Similar conclusions were recently obtained for the intersubband optical matrix elements [8]. We recently implemented the BF Hamiltonian for a triangular GaAs/AlAs (001) QWR with wire axis in the [001] direction and showed that there are differences of up to 10 meV for a baseline of 10 nm [9]. The V-groove QWR's grown have a wire axis along the $[1\bar{1}0]$ direction. It remains to prove that there can be a significant difference between the BF and LK calculations for such a structure and geometry. We, therefore, derived the BF Hamiltonian for a QWR along the $[1\bar{1}0]$ direction and carried out calculations for both GaAs/AlGaAs and InGaAs/InP QWR's. V-groove QWR's of InGaAs with {111}A InP facets and on (001) oriented InP:S substrates have also been grown by low-pressure MOCVD [10].

2 GEOMETRY OF QWR's

The actual geometry of the V-groove QWR's is fairly complicated and, thus, complete information is not available from the published literature. The most detailed description can be found in [1]. The overall structure is that of a crescent-shaped QWR with QW sidearms and accompanied by two vertical QW's that have an inverted Y structure (see Fig. 1 of [1]). Here we report comparisons for the 2.5 nm QWR for which the experimental shape is available [2] (Fig. 1).

3 THEORY

We have derived the BF Hamiltonian for a QWR with $[1\bar{1}0]$ wire axis. We will take as starting matrix the D matrix of Stravinou and van Dalen [11]. One can break down the process of obtaining the Hamiltonian in the new rotated coordinate system into three steps.

The first step involves rotating the basis functions of the three-band Hamiltonian. The second involves replacing the unprimed (unrotated) wave vector by the primed (rotated) one. The third involves re-expressing the matrix in terms of the coupled angular momentum JM states. One can give a succinct presentation of the procedure. Given

$$x'_j = U_{ji} x_i, \;\; k'_j = U_{ji} k_i, \tag{1}$$

and the original unrotated three-band Hamiltonian matrix

$$D_{\alpha\beta}(\mathbf{k}) = \sum_{ij} D^{ij}_{\alpha\beta} k_i k_j,$$

then, the first two steps lead to

$$D'_{\alpha'\beta'}(\mathbf{k}') = \sum_{\alpha\beta} \sum_{ij} \sum_{i'j'} U_{\alpha'\alpha} U_{\beta'\beta} U_{i'i} U_{j'j} D^{ij}_{\alpha\beta} k_{i'} k_{j'}. \tag{2}$$

This results in the matrix given in Table 1. A, B, C_1 and C_2 are as defined in [11]:

$$\begin{aligned} A &= 1 - 6\sigma - 12\delta = -(\gamma_1 + 4\gamma_2), \\ B &= 1 - 6\pi = -(\gamma_1 - 2\gamma_2), \\ C_1 &= 6\delta - 6\sigma = 1 + \gamma_1 - 2\gamma_2 - 6\gamma_3, \\ C_2 &= 6\pi = 1 + \gamma_1 - 2\gamma_2, \end{aligned} \tag{3}$$

where σ, π, δ are the Foreman parameters [6] reflecting the interaction of the valence states with atomic-like s, p, d states, and the γ_i's are the usual Luttinger parameters. The final step of converting to JM states will not be written out explicitly. One significant difference between the BF and LK Hamiltonians is the presence of an additional interaction between light-hole states of opposite spin and denoted by the matrix element C; a similar difference is present in the quantum-well Hamiltonian [6], [11].

Table 1: Stravinou and van Dalen Hamiltonian in $[1\bar{1}0]$ rotated LS basis.

$$D'(\mathbf{k}') = \frac{\hbar^2}{2m_0} \begin{array}{c} \\ |X'\rangle \\ |Y'\rangle \\ |Z'\rangle \end{array} \overbrace{\begin{pmatrix} k'_x A k'_x + k'_y B k'_y + k'_z B k'_z & k'_y C_1 k'_x - k'_x C_2 k'_y & k'_z C_1 k'_x - k'_x C_2 k'_z \\ k'_x C_1 k'_y - k'_y C_2 k'_x & \frac{1}{2}[k'_y(A + B + C_1 - C_2)k'_y + k'_z(A + B - C_1 - C_2)k'_z] + k'_x B k'_x & \frac{1}{2}[k'_z(A - B + C_1 + C_2)k'_y] \\ k'_x C_1 k'_z - k'_z C_2 k'_x & \frac{1}{2}[k'_y(A - B + C_1 + C_2)k'_y] & \frac{1}{2}[k'_y(A + B - C_1 - C_2)k'_y + k'_z(A + B + C_1 - C_2)k'_z] + k'_x B k'_x \end{pmatrix}}^{\begin{array}{ccc} |X'\rangle & |Y'\rangle & |Z'\rangle \end{array}}$$

4 ANALYSIS

Analysis of the resulting Hamiltonian reveals a number of interesting results.

4.1 Zone-center Energies

First, there can be a difference between LK and BF energies even at the Brillouin zone center. This is a new result not present in previous studies on quantum wells. However, at the zone center of the first Brillouin zone, all the off-diagonal matrix elements of the BF and LK Hamiltonians are the same. Furthermore, the Luttinger parameters between GaAs and $Al_{0.3}Ga_{0.7}As$ are

not very different, but there are substantial differences between $In_{0.53}Ga_{0.47}As$ and InP (Table 2). Together, these suggest that there might only be a small difference between the BF and LK energies for GaAs/AlGaAs but larger for InGaAs/InP QWR's.

Table 2: Luttinger parameters.

	γ_1	γ_2	γ_3
GaAs [12]	6.85	2.10	2.90
AlAs [12]	3.45	0.68	1.29
InAs [13]	20.4	8.3	9.1
InP [13]	4.95	1.65	2.35
$In_{0.53}Ga_{0.47}As$	14.03	5.39	6.19

4.2 Boundary Conditions

The standard technique is to integrate the differential equations across an interface. In the process, contributions arise from, for example, $\widehat{k}'_i \mathcal{A}(\mathbf{r}')f(\mathbf{r}')$ terms, where $\mathcal{A}(\mathbf{r}')$ are position-dependent material parameters (within LK theory, they are related to the Luttinger parameters) and $f(\mathbf{r}')$ is the envelope function. For quantum wells, this corresponds to the term $\widehat{k}'_z \mathcal{A}(z')f(z')$; when applied to the interaction between heavy-hole and light-hole states of the same spin, it only leads to π and δ contributions using the BF Hamiltonian [11], but it also includes the σ contribution if the LK Hamiltonian is used. In the QWR case, the same matrix element contains the term $\widehat{k}'_x C_1 f(z')$ which includes the σ contribution; this is the s-like coupling term absent from previous implementations of the BF theory, but which is present in the LK theory [6]. One can similarly analyze the other matrix elements. Overall, one expects that, at finite k_z the difference between BF and LK might be reduced.

5 NUMERICAL RESULTS

The above analysis was tested with a numerical implementation of the problem using a finite-element algorithm for solving the coupled partial differential equations.

For GaAs/AlGaAs, we obtained energy differences of < 1 meV for the small wave vector values relevant to the experimental data (Fig. 2). We further verified that this is due to the wire orientation by finding a small difference of < 1 meV for the same triangular wire we used in [9] (for which there were differences of order 10 meV between BF and LK energies when oriented along [001]) but now oriented along $[1\bar{1}0]$. This confirms that the effective difference between the BF and LK theories is reduced for the $[1\bar{1}0]$-oriented wire compared to [001].

The sum squared of the envelope-function components for the lowest electron and hole states are given in Fig. 1, showing the confinement of these states inside the QWR. The electron state was obtained using a one-band model.

We have also redone the above calculations for a lattice-matched $In_{0.53}Ga_{0.47}As$/InP QWR (Fig. 2). This system is chosen because V-groove QWR's based upon these materials have also been made [10], though the experimental structures are probably all strained. It is also interesting because there is a larger difference in the Luttinger parameters. Indeed, this translates into a correspondingly larger difference in LK and BF results (Fig. 2).

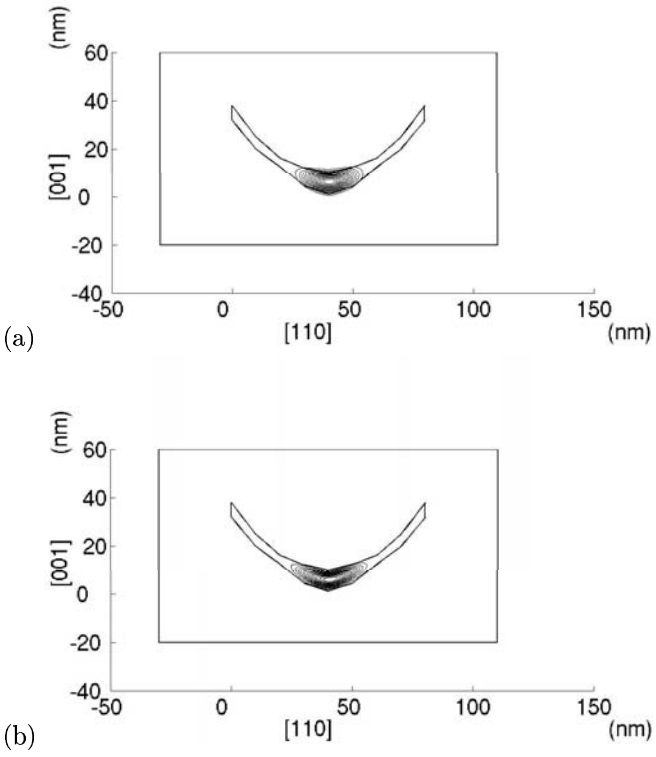

Figure 1: Geometry of embedded wire and first (a) electron, (b) hole probability density for the GaAs/AlGaAs QWR.

6 CONCLUSIONS

It is, therefore, concluded that the discrepancy between theory and experiment for GaAs/AlGaAs V-groove QWR's is not due to the use of the Luttinger-Kohn Hamiltonian. Possible reasons for the differences are excitonic binding energies, differences (both in geometry and composition) between the real and modeled structures, and the Luttinger parameters are not exactly known. On the other hand, InGaAs/InP QWR's have a better potential of revealing differences between the Luttinger-Kohn and the Burt-Foreman Hamiltonians.

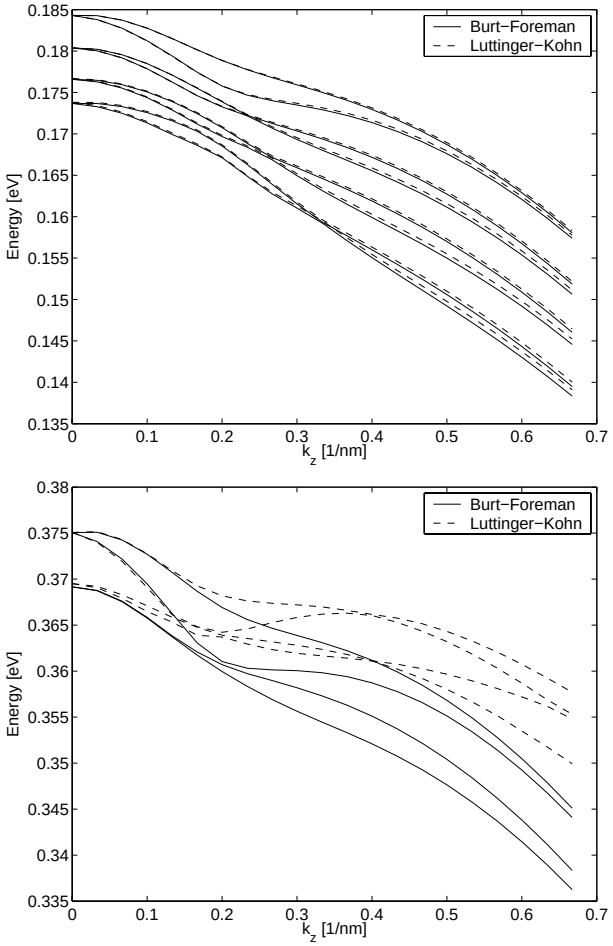

Figure 2: Valence band structure for 2.5 nm wire using BF (lines) and LK (crosses) Hamiltonians. Top (bottom) for GaAs/AlGaAs (InGaAs/InP).

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