Behavior of zone-center, subband energies in narrow, strongly coupled quantum wells

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Narrow, symmetric coupled quantum wells (CQWs) are studied using a $k \cdot p$, pseudopotential method. GaAs wells that range in width from 11.4 to 99.0 Å and $Al_{0.3}Ga_{0.7}As$ barriers that range in width from 11.4 to 17.0 Å are treated. Features of the systems such as energy positions as a function of well and barrier width, subband crossing, and subband splitting about the single well subband position are described. A simple function with subband-dependent constants is fit to both the subband-pair splitting as a function of barrier width and the subband energy position as a function of well width. This function provides an accurate and simple aid in CQW design for devices and experiments.

Coupled quantum well structures have recently attracted a great deal of interest due to the flexibility they provide for experimental and device applications.[1] Coupled quantum wells (CQWs) have also been found to be useful structures in which to study the quantum-confined Stark effect.[2] CQWs with thin barriers exhibit complex valance band structure, particularly when the wells themselves are also somewhat narrow. Band crossing due to subband splitting has been predicted and observed with[3] and without[4] an applied electric field.

In this letter we present the results of a theoretical study of zone-center subband energy positions for a range of well and barrier widths in CQWs. These results provide insight on a fundamental level into subband behavior and could aid in quantum well design for both applications and devices. A variety of symmetric CQWs are characterized using a $k \cdot p$, pseudopotential method based on that of Smith and Mailhiot.[5] In this formalism, effective masses and basis states are not assumed in each bulk material, but follow from the material parameters and the superlattice symmetry. Using a reference Hamiltonian, we find a single basis set for the constituent materials by a zone-center pseudopotential calculation. The Γ_1 conduction and the Γ_{15} valence states are coupled with a spinor and treated explicitly. Neighboring states are treated in Lowdin perturbation theory with the $\mathbf{k} \cdot \mathbf{p}$ operator, the perturbation being the difference between the material and reference pseudopotentials. The normal component of the current density operator is used for interface matching of the bulk material eigenfunctions.

The symmetric CQWs are modeled using a four-layer periodic structure consisting of two GaAs layers ranging in thickness from 4 to 35 atomic monolayers, 11.3 to 99.0 Å, separated by $Al_{0.3}Ga_{0.7}As$ barriers ranging in thickness from 4 to 6 atomic monolayers, 11.3 to 17.0 Å, with a thick $Al_{0.3}Ga_{0.7}As$ buffer layer to isolate the CQWs so that coupling occurs only through the thin barrier. This is shown in the inset of Fig. 1. The band-gap offset is divided, with 43% going to the valence band, and 57% going to the conduction band. Also, the growth direction of the CQWs is along one of the three principal axes of the unit cells of the bulk material. Calculations are done for systems at room temperature.

A number of useful insights are gained by considering the zone-center energy values of the first three valence subbands as a function of well width. Figure 1 shows these energy values over the range of well widths studied, for a barrier width of 11.4 Å. We find similar results for barrier widths of 14.1 and 17.0 Å. The heavy hole (HH1) and light hole (LH1) subbands are symmetric solutions and the HH2 subband is an antisymmetric solution, all of which arise when a single well subband is split by the coupling between two wells. The top of the GaAs bulk valence band is the zero of energy. It is seen that the LH1 subband crosses over the HH2 subband for a well width of 19.8 Å for the case shown in Fig. 1. This crossover occurs at well widths of 15.6 and 13.3 Å for barrier widths of 14. 1 and 17.0 Å, respectively. By noting the amount which the LH1 band moves beneath the HH2 band and approaches the HH1 band, it is seen that the LH1 band will not cross the HH1 band. This is in agreement with the limiting case of the barrier width going to zero. The two coupled wells then become a single well of twice the width and the first hole subband would be heavy hole-like. However, it is seen that for narrow wells and barriers, the LH1

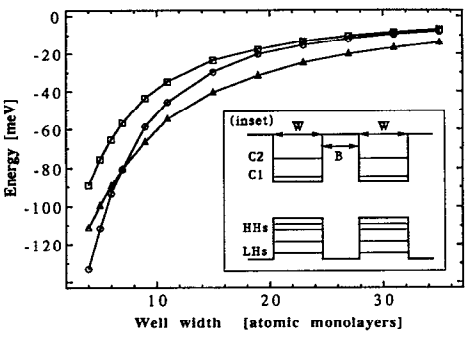

FIG. 1. Valence-subband energy position vs well width. GaAs wells are equal in width and run from 4 to 35 atomic monolayers, 11.4 to 99.0 Å in width. $Al_{0.3}Ga_{0.7}As$ barrier width is 11.4 Å. Energy zero is the top of GaAs bulk valence band (□) heavy hole, 1 (○) heavy hole 2, (△) light hole 1. (inset) Schematic diagram of system being considered. $Al_{0.3}Ga_{0.7}As$ barrier width, B, runs from 11.4 to 17.0 Å. GaAs well widths, W, run from 11.4 to 99.0 Å.

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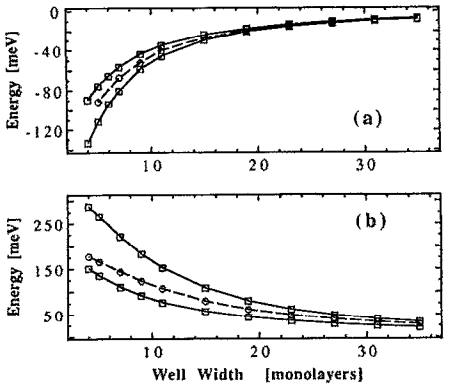

FIG. 2. (a) First heavy hole subband pair energies compared to single quantum well heavy hole energies [coupled well energy positions: (□), single well states: (○)]. Energy zero is bulk GaAs valence-band top. $Al_{0.3}Ga_{0.7}As$ barrier is 11.4 Å wide. (b) First electron subband pair energies compared to single well electron 1 energies [coupled well energy positions: (□) single well states: (○)]. Energy zero is bulk GaAs conduction-band bottom. Barrier is as in (a).

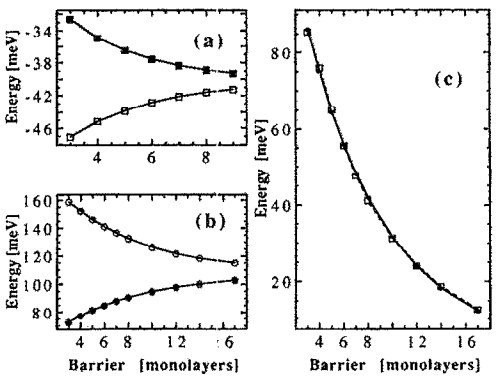

FIG. 3. (a) HH1 (■) and HH2 (□) energies vs $Al_{0.3}Ga_{0.7}As$ barrier width. GaAs wells are 31.1 Å wide. The energy zero is GaAs bulk valence top. (b) $C1$ (●) and $C2$ (○) energies vs $Al_{0.3}Ga_{0.7}As$ barrier width. Wells are the same as (a). The energy zero is GaAs bulk conduction bottom. (c) First conduction-band pair separation vs $Al_{0.3}Ga_{0.7}As$ barrier width. The wells are the same as (a). Barely detectable difference between results (circles, solid line) and fit (squares, dashed line).

subband is closer to the HH1 band than the HH2 band. These relative subband positions could play a useful role as a starting point in quantum-confined Stark effect based experiments or devices. Additionally, by extending the results given in Fig. 1 to the limit of zero well width, one sees that the HH1 and LH1 subbands approach each other and become degenerate. This is expected, since the zero well width case is merely bulk $Al_{0.3}Ga_{0.7}As$.

It is sometimes assumed that the splitting of the symmetric and antisymmetric subbands in CQWs is even about the single well subband position. This is not always true, as can be seen in Fig. 2, where the energy positions of the first heavy hole and conduction subband pairs are plotted, along with their equivalent single well subband energy positions. The unequal splitting arises because the narrow barrier allows for strong coupling between the wells, and hence causes the symmetric and antisymmetric subbands to split far apart. As the wells get very narrow, the HH1 and $C1$ subbands are forced so far "down" relative to their single well positions that the bottom of the well, the bulk band edge, literally "pushes" them away toward their single well positions. This can be seen in the way the antisymmetric HH2 and $C2$ subbands, unhampered by the well bottom, always move further from the single well HH1 and $C1$ positions as the wells narrow, whereas the coupled well HH1 and $C1$ reach a maximum separation from their single well positions and then move closer for narrow wells. One should note that the assumption of equal splitting about the single well subband position is still good when the barrier is high and wide enough and the wells are wide, enough.

The splitting of the first heavy hole and first conduction-band pairs as a function of barrier width is shown in Fig. 3. The splitting is greater for the conduction band than for the heavy hole because the coupling of the electron states through the barrier is stronger. This agrees with an effective mass argument for the different band types, the electrons being lighter and more mobile than the heavy holes. It was found that a function of the form

$$D=(A/x^2)+(B/x)+C \tag{1}$$

with D the energy splitting, A, B, and C, parameters which depend on the subband type and x the barrier width in monolayers, fits the data well for the barrier widths considered. The fit to the data is the dotted line in Fig. 3. This functional form is different from that proposed by Yariv *et al.*[6] for weak coupling situations, which has an exponential dependence on barrier width for the symmetric and antisymmetric subband energy splitting. The systems currently being considered are strongly coupled, especially the light hole and conduction subbands, since the barriers and wells are thin. The subband energy positions as a function a well width can also be fit using a function of this form. Here, D is the energy position and x is the well width in monolayers. The energy positions of the first and second heavy hole, first light hole, and the first and second electron subbands, with barrier widths of 11.4, 14.1, and 17.0 Å, are fit for well widths of from 11.3 to 99.0 Å. The values of A, B, and C are given in Table I for these cases. The fits are good for the systems considered. Hence, once the three parameters specific to each system are found, the energy position of that subband can be found generally and accurately. Note that A, the squared term constant, is much greater than B for the light holes and the conduction bands, while A and B are about equal for the heavy holes. This implies that the strongly coupled subbands have a stronger inverse well width squared component. The more weakly coupled heavy holes show a more linear dependence on the inverse well width. Yariv *et al.*[6] found a linear dependence on inverse well width for the subband splitting in weakly coupled cases. Since subband splitting as a function of well width is the difference between two subband positions, the functional form found here tends to agree with that of Yariv *et al.*

The fit begins to fail in certain regions. This occurs for the heavy hole subbands with wider well and barrier widths. When the wells are narrow, all types of subbands

TABLE I. Fitting parameters. Values of A, B, and C are given for Eq. (1) for the different subbands and barrier widths.

	A	B	C
11.4 Å barrier			
HH1	554.5	− 530.9	8.54
HH2	534.2	− 731.5	14.9
LH1	1330.0	− 806.6	7.73
$C1$	− 1918.0	1116.3	− 9.11
$C2$	− 4813.3	2491.1	− 35.8
14.1 Å barrier			
HH1	631.8	− 568.3	9.64
HH2	446.1	− 674.8	12.8
LH1	1491.2	− 855.8	7.66
17.0 Å barrier			
HH1	717.5	− 601.6	10.6
HH2	506.5	− 669.0	12.6
LH1	1618.7	− 892.7	7.71

exhibit the same functional dependence of their zone-center energies on well width. As the well widths increase, the heavy hole energies shift more slowly than the light hole or electron subband energies as a function of well width. This is understood by noting that when quantum confinement and coupling, that is the square-well nature of the system are the dominant effects driving subband energy position, all subbands will act the same. As the bulk properties of the constituent materials become more important, the specific subband type will gain importance in determining the subband location. Heavy holes are the least sensitive to quantum confinement and coupling, so they should be the first to show the influence of bulk material effects. This is the case here. Light holes and electrons continue to be dominated by quantum confinement and coupling for at least 100 Å well widths with these barriers, and thus, maintain the same functional form. However, the heavy holes go into a region in which bulk material parameters begin to play a significant role.

In conclusion, a study of the subband zone-center energy positions as a function of well and barrier width for a variety of narrow, strongly coupled quantum wells is presented. Interesting features of the subband energy positions, such as the crossover of the HH2 and LH1 subbands for narrow well and barrier widths, have been discussed with attention to the type of systems which will show these features. A region exists in which the assumption of even splitting of the symmetric and antisymmetric subband pairs about their single well positions is invalid. This arises largely due to the approach of the symmetric subband to the bottom of the well. A simple function, with subband-dependent parameters, was fit to both the subband splitting as a function of barrier width and the subband position as a function of well width. This simple result is useful in the design of CQWs for both experimental and device applications that require an accurate knowledge of subband positions, since the energy splittings and positions can be found accurately for a range of both barrier and well widths using the same functional form and without recourse to more complicated schemes. The accurate determination of the HH2 and LH1 crossover gives additional control in systems which depend on the relative positions of the heavy and light holes, such as optically bistable devices and systems which study or use the quantum-confined Stark effect.

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