

Electronic States in Quantum Wells With Non-Abrupt Interfaces

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We calculate the energy values and the spatial distributions of the bound electronic states in some quantum wells with graded interfaces. The calculations are performed within a sp^3s^* spin dependent empirical tight binding model. A good agreement is found between our calculations and experimental measurements for $AlGaAs/GaAs$ quantum wells with thermally induced changes in the profile at the interfaces. The theoretical results show that the transition ($C3-HH3$) is not sensitive to the diffusion length L_D , but the transitions ($C1-HH1$), ($C1-LH1$), ($C2-HH2$) and ($C2-LH2$) display large “blue shifts” with increasing L_D . The observed dependence is explained in terms of the bound states spatial distributions.

1. Introduction

The $Al_xGa_{1-x}As/GaAs$ heterostructures have non-abrupt interfaces due to unwanted diffusion of Al and Ga across the heterojunctions. These graded interfaces could change the electronic and optical properties of the quantum well structures [1-5]. A detailed study about the diffusion influence on the quantum well electronic states could allow to control and use the new features these systems display. A comparison between calculated and measured transition energies permits diffusion coefficients determination for different temperatures [2,4]. Till now quantum wells with compositional grading at the interfaces were studied mainly using simple effective mass models [1,4]. We believe that realistic tight-binding calculations will give a new information for these systems as was illustrated in [5] for an $AlAs/GaAs$ quantum well with linear concentration profile at the interfaces.

In the present paper we study the influence of the diffusion length L_D on the optical transitions energies in an interdiffused $Al_{0.2}Ga_{0.8}As/GaAs$ quantum well with an as-grown well width of 100 Å. (See fig.1.) This well was fabricated and experimentally studied in Ref. [1]. The energies of the transitions ($C1-HH1$), ($C1-LH1$) and ($C2-HH2$) have been measured at temperature 2° K for $L_D=0, 18, 20, 28, 48.5$ and 66 Å after annealing at 950° C for different time durations. The Al composition across the well after the diffusion can be found from a formula widely used in the literature (see for instance Eq. (2) in Ref. [1]). We use an sp^3s^* spin dependent empirical tight binding model, the virtual crystal approximation, the surface Green function matching technique and an algorithm established and used to study inhomogeneous finite slabs [6-9]. For more details see [6] and the references therein.

2. Results and Discussion

We calculated the energies of the first three bound electron states $C1, C2, C3$ and the first five hole states $HH1, LH1, HH2, LH2$ and $HH3$ in the quantum well under study for different diffusion lengths L_D . When L_D increases the bound states depart further from the $GaAs$ band edges.

Qualitatively similar results have been reported in [5] for

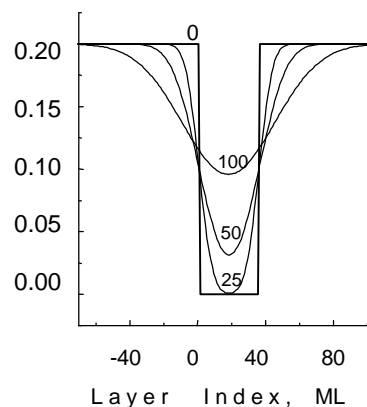


Fig.1. Quantum wells concentration profiles for different diffusion lengths (in Å).

an $AlAs/GaAs$ quantum well with linearly graded interfaces. As a difference from [5], in our case the energies of the states $C3, HH3$ and $LH2$ change several times less than the energies of the states $C1, C2, HH1, HH2$ and $LH1$.

In fig.2a are shown the theoretical curves of the transition energies dependence on the diffusion length L_D for the transitions ($C1-HH1$), ($C1-LH1$), ($C2-HH2$), ($C2-LH2$) and ($C3-HH3$) in $Al_{0.2}Ga_{0.8}As/GaAs$ diffused quantum wells. There is a “blue shift” for all transitions with increasing L_D as reported in [2,4] for similar systems. This shift is 27 meV for ($C3-HH3$) and 97 meV for ($C1-HH1$) when L_D increases from 0 to 70 Å. The transitions ($C1-HH1$), ($C2-HH2$), and ($C2-LH2$) shift with 94 meV, 82 meV and 65 meV respectively.

To understand the above mentioned dependencies we calculated the spatial distributions of all bound states for all diffusion lengths. If the Al concentration in the initial well region increases, the well effectively narrows and consequently the bound states energies in the diffused quantum well increase. On contrary, an Al concentration decreasing outside the initial quantum well broadens effectively the well and the energies of the bound states decrease. (See fig.1.) The transition ($C3-HH3$) is not

sensitive to the diffusion length for $L_D=20\div 100$ Å because the states $C3$ and $HH3$ spread over both regions affected from the diffusion (within and outside the initial well).

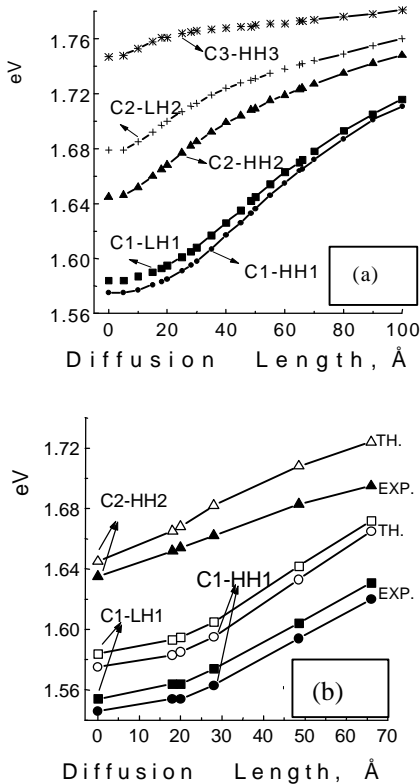


Fig.2. Transition energy dependence on the diffusion length.
a/ theory b/ theory and experiment.

The transitions ($C1-HH1$), ($C1-LH1$) and ($C2-HH2$) show considerable “blue shifts” in the interval $L_D=20\div 100$ Å because the spatial distributions of the states $C1$, $C2$, $HH1$, $LH1$ and $HH2$ are localized mainly in the region with increased Al concentration after the diffusion. A relatively low sensitivity of the transition ($C3-HH3$) to the diffusion length was measured in [2]. For low diffusion length values ($L_D \leq 20$ Å) the transition ($C3-HH3$) is sensitive to the L_D changes because then the Al concentration changes only around the interfaces where the states $C3$ and $HH3$ possess considerable spectral strengths. In this diffusion lengths interval the states $C1$, $C2$, $HH1$, $LH1$ and $HH2$ are less sensitive to the L_D changes due to the accumulation of these states mainly in the central well part where the Al concentration is not affected after the diffusion.

In fig. 2b we compare our theoretical curves with the experimental curves from [1] for ($C1-HH1$), ($C1-LH1$) and ($C2-HH2$) transitions energies with $L_D=0, 18, 20, 28, 48.5$ and 66 Å. The measurements in [1] have been conducted at temperature 2° K and temperature corrections of the theoretical values were not necessary. It is clear that the agreement with the experimental data is quite satisfactory taking into account that the calculations do not include excitonic effects and that we have made no fit.

All experimental curves lie below the theoretical ones with a displacement of $10\div 45$ meV. The agreement between the theory and the experiment is better for the excited states than the ground states due to the fact that the exciton binding energies are higher for the ground states. The curves in fig.2b diverge for all transitions with L_D increasing. For instance, the differences are 29 meV, 30 meV and 10 meV for ($C1-HH1$), ($C1-LH1$) and ($C2-HH2$) respectively with $L_D=0$ Å and 45 meV, 41 meV and 29 meV with $L_D=66$ Å. A possible explanation of this behaviour could be an increasing of the excitonic binding energy for higher L_D values due to the higher Al concentration within the initial well region. This means that even for $L_D=66$ Å the excitations are localized. The spatial distributions of the bound states for these diffusion lengths support such an assumption. An exciton binding energy increasing has been reported [4] in double-barrier quantum wells when L_D increases.

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