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$^3$s* 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 of 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$_x$Ga$_{1-x}$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 matching technique and an algorithm established and used to control and use the new features these systems display. A good agreement is found between our calculations and experimental measurements for AlGaAs/GaAs quantum wells 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$_{x}$Ga$_{1-x}$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$^3$s* 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] sand 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 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 broads 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 \( L_D = 20 \pm 100 \) Å because the states C3 and HH3 spread over both regions affected from the diffusion (within and outside the initial well).

![Fig. 2](image)

**Fig. 2.** Transition energy dependence on the diffusion length.

(a) theory  
(b) theory and experiment.

All experimental curves lie below the theoretical ones with a displacement of 10±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. Some data [4] in double-barrier quantum wells when \( L_D \) increases.

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