Electronic states in parabolic versus diffused quantum wells

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Numerical calculations are performed to determine the energies of the electronic bound states in parabolic and diffused quantum wells. A comparison of the electronic spectra for these concentration profiles is made and equidistant energy levels for a diffused quantum well are found. The virtual crystal approximation and the surface Green function matching (SGFM) method are used within the framework of a semi-empirical \( sp_{3s}^* \) spin-dependent tight binding model.

Keywords: Quantum wells; diffusion

To calculate the energy spectra of the quantum wells we have applied the surface Green function matching (SGFM) method [8], the \( sp_{3s}^* \) spin-dependent tight binding model [9] and the virtual crystal approximation. This latter approach is explained in [10]. Previous tight binding calculations of electronic and optical properties in diffused quantum wells [10, 11] and complex heterostructures [12, 13] have given reliable results comparing with experimental data.

1. Introduction

The most important feature of the energy spectrum in parabolic quantum wells is the equidistance between the energy levels [1]. But it is not so easy to grow a quantum well with a parabolic concentration profile. Two different approaches are mainly used, the analog alloy method [2, 3] and the digital alloy method [3, 4]. The first approach is technically very complicated and the second one has the limitations of the digital approximation.

Some calculations [5] and measurements [6] have indicated that an interdiffused AlGaAs/GaAs quantum well may possess an energy spectrum very similar to the energy spectrum of a parabolic well. One can control the interdiffusion process by means of the sample temperature and different time durations of the annealing procedure [7]. So, an alternative way to grow a quantum well with equidistant energy level exists. Further considerations are needed to clarify this possibility. In the present work we try to make a first step in this direction.

2. Model

We have studied AlGaAs/GaAs quantum wells grown in (001) direction. The center of the two-dimensional Brillouin zone is considered. Two different parabolic wells and one diffused well have similar concentration profiles (see Figs. 1a and 1b).

Se calculan las energías de los estados ligados en pozos cuánticos parabólicos y con difusión. Se comparan los espectros de estos pozos con perfiles diferentes de la concentración y se encontraron niveles equidistantes en el pozo con difusión. Se usan la aproximación del cristal virtual, el método de empalme de las funciones de Green superficiales y un modelo de enlace fuerte semi-empírico \( sp_{3s}^* \) con espín.

Descriptores: Pozos cuánticos; difusión

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FIGURE 1. Al concentration profiles in diffused and parabolic quantum wells. Diffused QW: the well width of the as grown rectangular QW $L_w = 35$ MLs (10 nm), the diffusion length $L_D = 10$ nm (35 MLs), the Al concentration in the barrier before the diffusion $C_b = 0.2$, the Al concentration in the well before the diffusion $C_w = 0.1$, the well width of the diffused QW $L_w (DQW) = 201$ MLs (56.8 nm). Parabolic QWs: (a) PQW1, the Al concentration in the barrier $C_b = 0.2$, the Al concentration in the center of the well $C_w = 0.1$, the width of the parabolic QW1, $L_w (PQW) = 201$ MLs (56.8 nm). (b) PQW2, $C_b = 0.2$, $C_w = 0.095$, $L_w (PQW) = 201$ MLs (56.8 nm).

4. Conclusion

The results that we have obtained show the similarity of the energy spectra in parabolic and diffused quantum wells. A better fit to the concentration profile curves before the energy spectra calculation could improve the equidistance of the energy levels for the diffused well. It is easier to change the concentration profile of an as grown rectangular QW by means of thermal diffusion than to grow a parabolic QW. Further studies are needed to establish an annealing procedure for different temperatures and annealing times.

FIGURE 2. Energies of the electron bound states in diffused and parabolic quantum wells versus the main quantum number $n$. The zero of the energy scale is at the top of the AlAs valence band. (a) Electronic states $C_n$, $n = 1, 2, 3, 4, 5$. (b) Heavy hole states $HH_n$, $n = 1, 2, 3, 4, 5$. (c) Light hole states $LH_n$, $n = 1, 2, 3, 4$. 

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FIGURE 3. Energies of the transitions between the bound states in diffused and parabolic quantum wells versus the main quantum number \( n \).

(a) Transitions \( (C_n-HH_n) \), \( n = 1, 2, 3, 4, 5 \).
(b) Transitions \( (C_n-LH_n) \), \( n = 1, 2, 3, 4 \).

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