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SEMICONDUCTOR QUANTUM WELLS IN A CONSTANT ELECTRIC FIELD

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ABSTRACT
Electron and hole states in semiconductor nanostructures (quantum wells) exposed to electric field perpendicular to the layers have been calculated as well as the energies of the main optical transitions without and with applying a constant electric field. The quantum wells under study are of rectangular and graded composition quantum well structures - parabolic and linear. The aim of this study is the comparison of these quantum wells in the presence of an electric field. A comparison with the theoretical results and the experimental data available for these quantum wells has been made.

Key words: graded gap quantum wells, rectangular quantum wells, AlGaAs/GaAs, electric field effect, electron states, Stark effect.

INTRODUCTION

This work is motivated by the tremendous interest in the semiconductor nanostructures [1-2]. This interest is due to their actual and potential applications in various electro-optical devices. The effect of an external constant electric field on electron states (quantum confined Stark effect) in semiconductor quantum well (QW) structures and its many manifestations are of great interest due to the fact that most of the devices based on QWs work under application of an electric field [2-5]. Of particular interest for device applications are the magnitude of the field induced changes in the energy levels and localization of the wave function in QWs. The aim of the present study is to carry out realistic semi-empirical tight-binding (TB) calculations for the longitudinal quantum confined Stark effect in rectangular quantum wells (RQWs) with different thicknesses. We compare our results with those obtained by us previously for graded-gap QWs of parabolic [3] and linear [4] concentration profiles. The comparison of the results is made also with the experimental data and other calculations for the QWs with similar parameters [6-11].

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MODEL AND METHOD

The QWs under study are of the type GaAs./ $Al_xGa_{1-x}As$. We study RQWs of GaAs with three different thicknesses of 11 MLs, 22 MLs and 44 MLs. One ML (monolayer) equals two atomic layers and 1ML equals 2.825×10^{-10}m. We compare our results for RQW of 44 MLs with our previously results for parabolic QW (LQW) [3] and linear QW (PQW) [4] of the same width. The Al concentration x in the barriers $Al_xGa_{1-x}As$ is x = 0.36 for all QWs. In the RQW x is x=0. In the PQW x varies parabolically from 0.02 at the barriers to 0.12 in the middle of the well. In the LQW x varies linearly with n from 0.02 at the left edge to 0.36 at the right one. The Al concentration x is a constant in every layer, but is a function of n. The calculations are made for the temperature T = 0 K. We calculate the electron bound states and the hole bound states without and with applying a constant electric field F. The electric field F is applied parallel to the growth axis [001]. The cation is in n = 1. In the barrier regions the field is F = 0 for all QWs. We calculate also the energies of the main optical transitions *E(C1-HH1)*, *E(C1-LH1)*, *E(C2-HH2)* and their Stark (electric field) shifts. The

Stark shift consists of a decrease of the energy of a given optical transition in a QW when an electric field is applied.

Numerical calculations are made by the semi-empirical tight-binding approximation in the spin dependent sp^3s^* basis, the virtual crystal approximation and the surface Green function matching method. We use it as it is described in [12]. We define the presence of an external static electric field by adding a linearly varying with the distance term Δ_n to the diagonal elements of the TB Hamiltonian matrix:

$TB(n, x) = TB(x) + \Delta_n$,
$\Delta_n = (n - 1) \cdot F \cdot a/4$, where

a is the lattice constant, F - the intensity of the longitudinal constant electric field, TB(x) - the diagonal TB parameters without an electric field for the bulk material with Al concentration x, n - the number of the layer (i.e. layer index) in QW. We define the TB parameters TB(x) of the alloy $Al_xGa_{1-x}As$ by the virtual crystal approximation:

$TB(x) = x \cdot TB(AlAs) + (1-x) \cdot TB(GaAs)$.

The electric field is applied between the two sides of the QW. It is positive if it moves down the right side of the conduction band edge.

RESULTS AND DISCUSSION

Figure 1 displays the calculated ground state energies of the conduction *C1* and valence *HH1* states in the three rectangular QWs versus the applied constant electric field. We notice that the electric field effects depend significantly on the well width: at the same value of the electric field F, the Stark shift increases with the width of the QW.

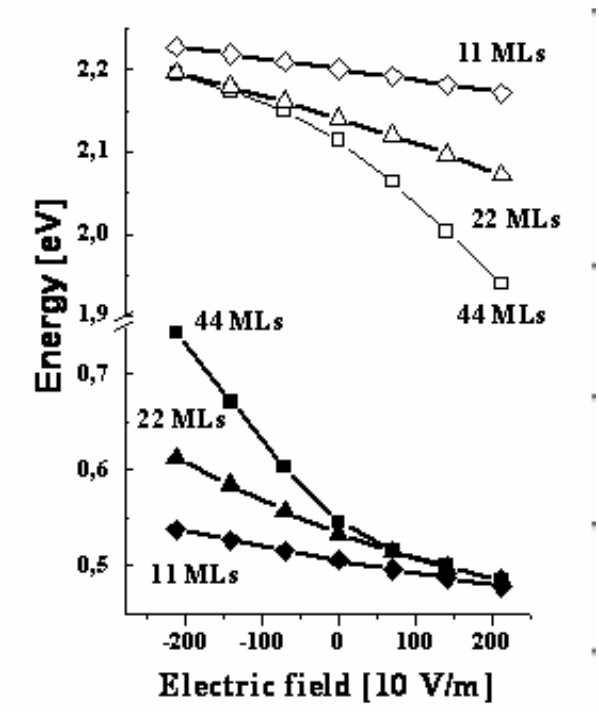

Figure 1. The ground state energies of the conduction *C1* (open symbols) and valence *HH1* (full symbols) states in RQWs with different widths: 11 MLs RQW - diamonds, 22 MLs RQW - triangles, 44 MLs RQW - squares.

Figure 2 shows the dependence of the main optical transition energy *E(C1-HH1)* from the electric field for the three RQWs. Here the similar dependence is observed: wider QW is, stronger influence of the electric field is. Increasing the applied electric field, the transition energy decreases.

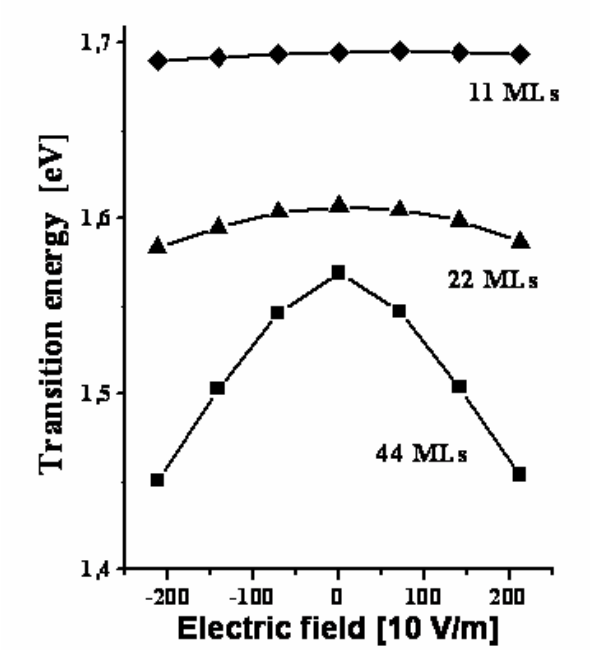

Figure 2. The dependence of the main optical transition energy *E(C1-HH1)* for the three RQWs (widths: 11, 22 and 44 MLs) on the applied electric field intensity.

Figure 3 shows the dependence of the main optical transition energies *E(C1-HH1), E(C1-LH1)* and *E(C2-HH2)* from the applied electric field for the three QWs of the same width of 44 MLs. On the figure (a) corresponds to the PQW case, (b) – to the LQW case, and (c) – to the RQW case. Here the similar dependence is observed: wider QW is, stronger influence of the electric field is. For the three QWs with increasing the applied electric field, the transition energies decrease. The transition energy *E(C1-HH1)* is larger in LQW than in RQW and than in PQW under application of the same *F*. The transition energies *E(C1-LH1)* and *E(C2-HH2)* are larger in the parabolic than in the rectangular and the linear QW at the same *F*, however they are larger in RQW than in LQW. A comparison of our calculations with the experimental data and other calculations for the QWs with similar parameters is presented in **Table 1.** There is a good correspondence between our calculated values and the experimental data sets presented in **Table 1**

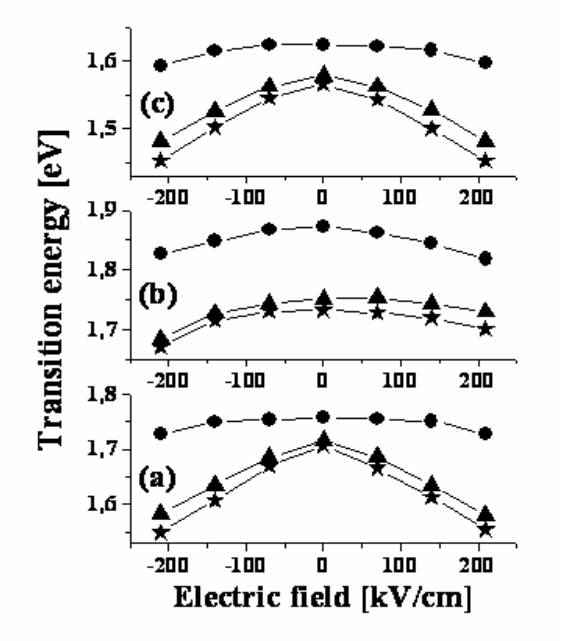

Figure 3. Transition energy as a function of applied electric field for PQW (a), LQW (b) and RQW (c): *E(C1-HH1)* - diamonds; *E(C1-LH1)* - squares; *E(C2-HH2)* - triangles.

Table 1. *A comparison of the calculated values with the values from the literature for the Stark shifts of E(C1-HH1) for RQWs.*

Stark shift of *E(C1-HH1)*, [10^{-3} eV]		This work			[6]		[7]		[8]	[9]	[10]	[11]
Field, [10 V/m]	70	1.00	2.00	24.00	0	6.00	0	7.10	20.00	10.00	7.36	8.09
	140	0	8.00	67.00	2.00	20.00	0	18.75				
QW width, [MLs]		11.00	22.00	44.00	17.70	35.40	17.70	35.40	46.02	35.40	36.11	35.40
x (Aluminium concentration in the barriers)		0.36			0.30		0.30		0.35	0.60	1.00	0.60

Some discrepancies can be due to the differences in the QW parameters (widths, barrier concentration profiles), temperature and excitonic effects. Note that our calculations do not include either temperature or excitonic effects.

The results we have obtained here demonstrate that the algorithm [7] with the appropriate parametrisation for the presence of the constant electric field works very good in practice and gives reasonable results for the RQWs, PQWs and LQWs.

CONCLUSIONS

Our calculations allow a detailed electronic structure investigation of QWs with different potential profiles in the presence of a constant electric field. A tight-binding study of these systems can give new information on the Stark effect. The TB method takes into account the real structure of the solid, many bands and their mixing together with the in-plane periodicity of the quantum well structure. The TB study of the Stark effect of the electronic states in the presence of electric field gives the possibility to look for a potential profile that provides good Stark effect characteristics of a given QW. Such calculations are very promising in looking for potential device applications, such as based on quantum confined Stark effect. The investigation of the electric field effects on the optical properties of the QW structures with graded-gap potential profiles is essential for the optimization of QW-based devices. The work is in progress in this direction.

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