A TIGHT-BINDING STUDY OF THE QUANTUM CONFINED STARK EFFECT IN SOME TRIANGULAR QUANTUM WELLS

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Abstract: *In this paper are calculated electronic and hole states in semiconductor quantum wells with variable chemical composition (graded-gap quantum wells), namely triangular quantum wells, with and without the application of a longitudinal constant electric field. The energies of the main optical transitions and their spatial distributions are calculated with and without the application of electric field. The aim of this work is the comparison of these quantum wells (that are the same width but with different inclinations of the linear concentration profile) in the presence of an electric field. A comparison with the available experimental data for these quantum wells has been made.*

ПРЕСМЯТАНЕ НА КВАНТОВО ОГРАНИЧЕНИЯ ЩАРК ЕФЕКТ С МЕТОДА НА СИЛНАТА ВРЪЗКА В НЯКОИ ТРИЪГЪЛНИ КВАНТОВИ ЯМИ

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Ключови думи: *Полупроводникови квантови ями, квантово ограничен Щарк ефект, метод на силната връзка, AlGaAs, електронни състояния, електрично поле, квантови ями с променлив химичен състав*

Резюме: *Пресметнати са електронните и дупчести състояния в полупроводникови квантови ями с променлив химичен състав, а именно триъгълни квантови ями, без и при прилагане на надлъжно постоянно електрично поле. Пресметнати са енергиите на основните оптични преходи с и без поле, както и пространствените им разпределения. Целта на работата е да се сравнят пресметнатите квантови ями, които са с еднаква ширина, но с различен наклон на линейния концентрационен профил в присъствието на постоянно електрично поле. Направено е сравнение с наличните експериментални данни за такива квантови ями.*

Introduction

In semiconductor quantum wells (QWs), sharp excitonic absorption peaks are clearly observed even at room temperature. When an electric field is applied perpendicular to the QW layers, the energy of the fundamental absorption edge shifts by a large amount without severe broadening of the exciton resonance. This is the well-known quantum confined Stark effect (QCSE). These properties enable one to utilize QWs for high-performance room temperature optoelectronic devices. Moreover, to improve the performance of these optical devices, band structure modifications in QWs have also been investigated. The electric field effects (Stark effects) on the graded-gap QW structures, where the band gap of the well is inclined along the growth direction, are one of the most promising among the modifications for applications of making various fast optoelectronic devices [1,2,3]. The modification of the well potential shape can create different optical properties and thus optimize nanostructure-based devices compared to conventional rectangular QWs (RQWs). The aim

of this study is to conduct numerical calculations with one of the methods, which is widely used for atomistic investigation of semiconductor nanostructures – the empirical tight binding method. Numerical calculations within the framework of a realistic tight-binding (TB) model for the electron and hole bound states of some semiconductor nanostructures, namely of asymmetric triangular quantum wells with different depths, in the presence of a constant electric field have been made.

Model and method

In this work we present the numerical calculations results of single quantum wells of the type $Al_xGa_{1-x}As$, with an asymmetric triangular concentration profile. This profile is realized by linear variation of the concentration within the well region. The electric field is applied parallel to the growth axis [001]. The three QWs under study have a width equal to 44 monolayers. One monolayer is equal to 2.825 x 10^{-10} m. The concentration x of Al in $Al_xGa_{1-x}As$ barrier for all of the wells is constant and equals to 0.36, i.e. all barriers are semiinfinite and with a composition $Al_{0.36}Ga_{0.64}As$. The concentration x of Al in the well varies linearly from 0.02 at the left edge of the well to 0.12 (QW1), 0.24 (QW2) and 0.36 (QW3) at the right edge of the well, respectively for the three considered QWs: QW1, QW2 and QW3, as shown schematically in Fig . 1. In Fig. 1 QWs are shown without applied electric field. The calculations are made for temperature T = 0 K.

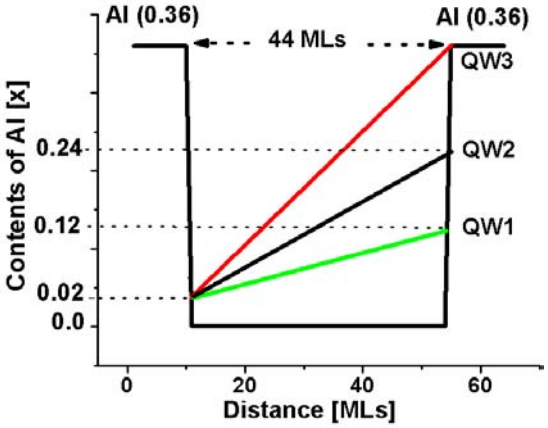

Fig. 1. Scheme band diagram of the three calculated quantum wells. The profiles of the contents x of Al is shown, it coincides with the potential energy profile of quantum well

We use the sp^3s^* spin-dependent semi-empirical tight-binding model as it is described in [4]. The virtual crystal approximation is used for the description of the TB parameters TB(x) of the alloy $Al_xGa_{1-x}As$:

TB(x)=x.TB(AlAs) + (1-x).

We use surface Green function matching technique, in order to calculate the Green function of the infinite system containing the finite inhomogenious slab. We define the presence of an external static electric field by adding an linearly varying with the distance term to the diagonal elements of the TB Hamiltonian matrix. This method allows also realistic TB calculations of the electronic states in quantum wells with variable concentration profile in the presence of a constant electric field (F) [5,6]. Electric fields are applied between the first and the last monolayer of the QW in the direction of crystal growth. In barrier areas in all QWs electric field is zero. All QWs have a width of N = 44 MLs. Everywhere direction of crystal growth [100].

Results

Tables 1, 2 and 3 show the all calculated main bound electron and hole energies of the three QWs under study without and in the presence of a constant electric field F. C1 and C2 are the conduction band bound states, and HH1, LH1 and HH2 are the valence band bound states. Some of this energies are partially investigated [7]. For all three QWs the behavior of the energies is similar: they decrease or increase with increasing or decreasing the applied electric field. We note the following dependence: the higher the content of Al in quantum well (QW3 has the highest content of Al), the higher is the value of the energy state in the conduction band, depending on the applied electric field. The above dependence is also valid for energies in the valence band.

Table 1. Main calculated bound electron (C1 and C2) and hole (LH – light holes and HH – heavy holes) energies (eV) for QW1 (see Fig. 1) without and with the application of a constant electric field F (kV/cm)

F [kV/cm]	C1 [eV]	C2	HH1	LH1	HH2
-212.4	2.228	2.328	0.689	0.665	0.638
-141.6	2.212	2.296	0.619	0.602	0.583
-70.8	2.193	2.259	0.555	0.545	0.537
0.0	2.169	2.216	0.515	0.504	0.493
70.8	2.135	2.172	0.495	0.478	0.455
141.6	2.085	2.130	0.480	0.459	0.427
212.4	2.025	2.088	0.468	0.444	0.403

Table 2. The same as in Table 1, but for QW2

F [kV/cm]	C1 [eV]	C2	HH1	LH1	HH2
-212.4	2.245	2.361	0.638	0.619	0.598
-141.6	2.231	2.334	0.571	0.560	0.549
-70.8	2.216	2.304	0.484	0.479	0.454
0.0	2.198	2.269	0.500	0.483	0.465
70.8	2.176	2.229	0.484	0.465	0.433
141.6	2.147	2.183	0.449	0.409	0.365
212.4	2.100	2.14	0.461	0.436	0.388

Table 3. The same as in Table 1, but for QW3

F [kV/cm]	C1 [eV]	C2	HH1	LH1	HH2
-212.4	2.260	2.389	0.588	0.577	0.563
-141.6	2.248	2.367	0.532	0.525	0.497
-70.8	2.235	2.340	0.505	0.492	0.475
0.0	2.220	2.312	0.489	0.470	0.442
70.8	2.203	2.278	0.475	0.454	0.416
141.6	2.182	2.239	0.464	0.440	0.394
212.4	2.156	2.194	0.455	0.428	0.375

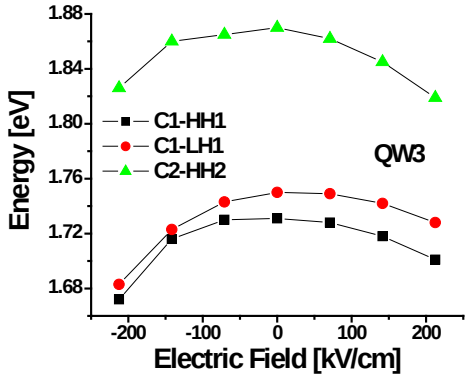

Fig. 2. Dependence of the main optical transitions from the applied electric field F for QW3. (C1-HH1) - rectangles, (C1-LH1) - circles and (C2-HH2) – triangles.

From Fig. 2 and the other data for QW1 and QW2, of the energies of the main optical transitions, we conclude that they are greatest in QW3 than in QW1 and QW2, at the same value of the applied field F.

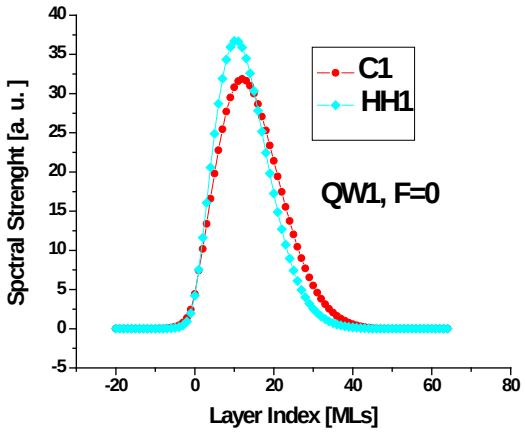

Fig. 3. Spatial distributions of the total spectral strength for C1 and HH1 states in QW1.
The electric field intensity F is zero.

We have calculated the total spectral strength spatial distributions for all states, corresponding to the energies given in tables 1-3. But for the lack of space we couldn't give them all here. In Fig. 4 are shown the results of the total spectral strength spatial distributions. The applied electric field intensity F is given on the picture. For the three QWs there is a complete overlap of the spatial distributions at F=0 kV/cm (see Fig. 3 for QW1). A displacement of the spatial distributions of C1, HH1 and LH1 states appears at electric field F≠0. It is larger for QW1 than for QW2 and QW3. Namely it is larger for QW with smaller Al content (most shallow). We can conclude that QW1 is not suitable for applications at such fields, as F very quickly moves the electrons and holes outside QW. On Fig. 4 we see that for QW2 and QW3 (see Fig. 5) the critical value of the electric field is achieved. Ai the critical value the intensity of the optical transition tends to zero due to the absence of spatial overlap between the states.

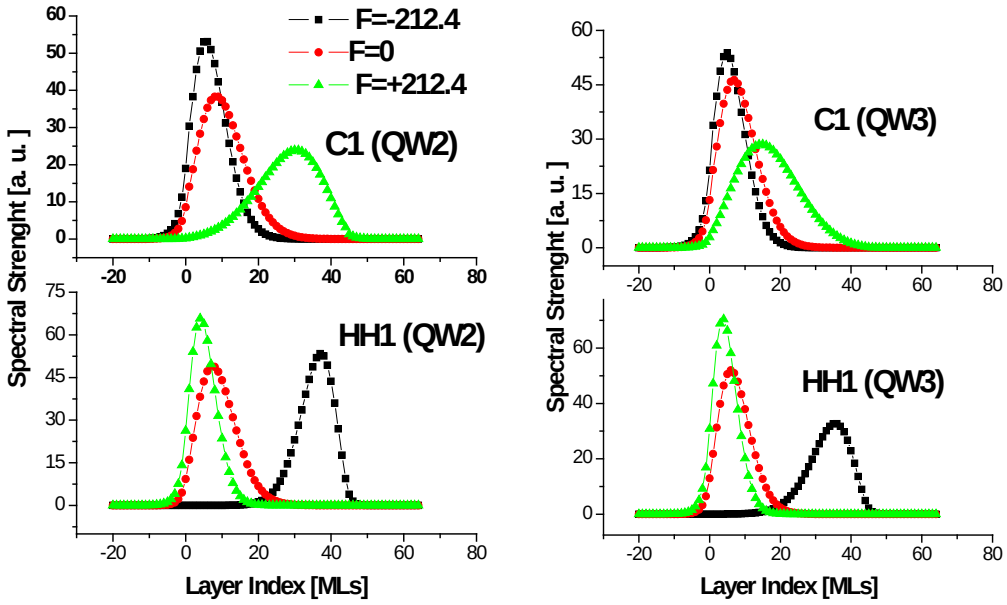

Fig. 4. Spatial distributions of the total spectral strength for C1 and HH1 states in QW2 and in QW3.
The electric field intensity F is given on the picture

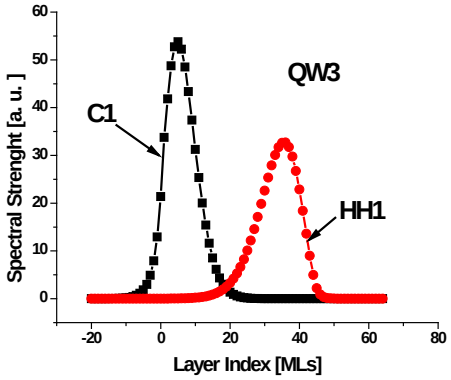

Fig. 5. Spatial distributions of the total spectral strength for C1 and HH1 states in QW3. The electric field intensity F is the critical value of the electric field

Concluding remarks

We may conclude that QW3 has the better Stark effect characteristics than QW2 and QW1. And also, the composition profile of QWs is essential in their Stark effect characteristics. The actual composition profiles of QWs, experimentally obtained, may differ significantly from those of the ideal QW stricture. Then a more realistic calculation would require taking account of the measured composition profile. With the method used here there would be no difficulty in taking in full account of any details of a realistic model that one might want to study. The work is in progress in this direction. Such investigations will help to find a QW potential profile with better Stark effect characteristics. 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.

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