ELECTRONIC SPECTRUM STUDY OF PARABOLIC $GaAs/Al_xGa_{1-x}As$ SUPERLATTICES

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Abstract—The electronic structure of finite parabolic $GaAs/Al_x Ga_{1-x}As$ superlattices is studied. A detailed analysis of the miniband formation is given and the importance of all system parameters is discussed. The dependence of the equidistant miniband separation on the superlattice size is revealed. A comparison with different theoretical methods and experimental data is presented. The calculations are conducted in the framework of the semi-empirical sp^3s^* tight-binding model including spin applying the Green function formalism and the Surface Green Function Matching Method (SGFM) method.

1. INTRODUCTION

The fast advancement in epitaxial growth techniques has permitted the construction of semiconductor layer systems with arbitrary potential profiles. In particular, the parabolic quantum well (PQW) [1], aside to the square one, is one of the most studied systems both from fundamental and technological points of view [2–7]. This is, partially, because its unique properties such as: equally spaced electronic spectrum, radiative transitions at the same oscillator frequency, interaction with light at the oscillator frequency irrespective of electron-electron interactions, i.e., independence on the number of electrons in the well and on an electric field applied across the well, the so called generalized Kohn theorem [8, 9].

Recently, PQW's have been implemented to study non-linear optical properties [10, 11], the quantum Hall effect [12, 13], charge and spin oscillations in 3D gases [14, 15], magnetic properties for the

spin electronics [16, 17], and band gap discontinuities in materials with outstanding characteristics [18, 19].

From the technological point of view, PQW's and PQW superlattices (PQWSL's) can be used as polarization insensitive electroabsorbative modulators [6] and far-infrared resonant tunneling devices [7]. Maranowski et al. [7] have demonstrated the radiative decay through multiple evenly spaced energy levels in PQWSL's as well as an efficient injection when a chirped superlattice acts as an electron filter replacing the barrier.

Here, the miniband structure formation in $GaAs/Al_xGa_{1-x}As$ parabolic quantum well superlattices within the spin-dependent sp^3s^* tight-binding semi-empirical model is considered. We study the miniband formation for electrons and holes of finite superlattices as a function of the system parameters, such as, the Al content, the well and barrier widths.

2. MODEL

The parabolic graded $GaAs/Al_xGa_{1-x}As$ superlattice is constructed as follows: a) a single parabolic well with three fundamental regions: left and right $Al_xGa_{1-x}As$ barriers of width d_B^L and d_B^R, and Al content x_L and x_R, respectively; $GaAs/Al_xGa_{1-x}As$ quantum well of width d_W and Al content varying parabolically from the left barrier (x_L) to the center ($x = 0$), and from the center to the right barrier (x_R); b) the single parabolic well of point a) is taken as period of the superlattice, so, the finite superlattice is obtained via N replicas of this period. In the present report the system is symmetrical, so, the left and right barriers are identical $x_L = x_R = x_B$. The next step is to embed the superlattice between two $Al_xGa_{1-x}As$ homogeneous barriers.

The electronic structure calculations are performed within the lines of the spin-dependent sp^3s^* tight-binding model and the surface Green function matching method [21, 22]. The Green function of the external barriers is calculated by means of the transfer matrix method in the usual way, and the Green function of the superlattice region is computed through an algorithm already used to study this kind of quantum structures [21–23].

All calculations are performed at the center of the two-dimensional Brillouin zone for the (001) growth direction.

3. RESULTS AND DISCUSSION

In Tables 1 and 2 the miniband structure formation for electrons and holes is presented for ten period PQWSL's. The Al barrier

Table 1. Conduction miniband-structure formation of ten period PQWSL's for $x_B = 0.21$. The barrier and well widths are given in ML's, while the energy in eV. The energy origin is taken at the top of the $AlAs$ valence band.

$d_B/2$	E_0		E_1
	$d_w = 30$	$d_w = 16$	$d_w = 30$
$SPQW$	2.155	2.196	2.255
100	2.155	2.196	2.255
40	2.155	2.196	2.255
30	2.155	2.196	2.255
20	2.155	2.196	2.255
10	2.155	2.196	2.255
5	2.155	$2.195 - 2.199$	$2.254 - 2.257$
2	2.155	$2.183 - 2.213$	$2.248 - 2.273$

Table 2. Valence miniband-structure formation of ten period PQWSL's for $x_B = 0.21$. The barrier and well widths are given in ML's, while the energy in eV. The energy origin is taken at the top of the $AlAs$ valence band.

$d_B/2$	E_0		E_1	
	$d_w = 30$	$d_w = 16$	$d_w = 30$	$d_w = 16$
$SPQW$	0.525	0.503	0.505	0.481
100	0.525	0.503	0.505	0.481
40	0.525	0.503	0.505	0.481
30	0.525	0.503	0.505	0.481
20	0.525	0.503	0.505	0.481
10	0.525	0.503	0.505	0.481
5	0.525	0.503	0.505	$0.488 - 0.469$
2	0.525	0.503	$0.508 - 0.506$	$0.494 - 0.449$

concentration is fixed at $x_B = 0.21$. We have considered barriers from 200 ML's to 4 ML's for two well widths, 30 ML's and 16 ML's. We also have included a single PQW (SPQW) as a reference system. The energy is given in eV. The energies are measured from the top of the $AlAs$ valence band. From Table 1 it is clear that for electrons there are two levels when $d_W = 30$ ML's, while when $d_W = 16$ ML's there is

only one. This is due to the stronger attractiveness as the well width is increased. PQWSL's behave practically like isolate PQW's from barrier widths of 200 ML's to 20 ML's, in both cases. An evident level splitting is presented for the ground electron level for $d_W = 16$ ML's and barrier widths of 10 ML's and 4 ML's, with energy-miniband width of 4 meV and 30 meV, respectively. For $d_W = 30$ ML's the level splitting is present at the same barrier widths as in the case of the electron ground level ($d_W = 16$ ML's), but for the first excited level. The corresponding energy-miniband widths are 3 meV and 25 meV, respectively. In the case of holes a similar trend is observed as the well width is increased, Table 2. The level splitting is presented only for the ground light hole state in both cases, $d_W = 30$ ML's and $d_W = 16$ ML's. The energy-miniband width is 2 meV for $d_W = 30$ ML's and $d_B = 4$ ML's, while for $d_W = 16$ ML's we have 19 meV and 45 meV for barrier widths of 10 ML's and 4 ML's, respectively.

In Fig. 1, we present the density of states of ten period PQWSL's for conduction ((a) and (c)) and valence ((b) and (d)) band with the following set of parameters: $d_W = 16$ ML's, $d_B = 4$ ML's, $x_B = 0.21$ ((a) and (b)) and $x_B = 0.30$ ((c) and (d)). We also include an isolated PQW for reference. We can see clearly the level splitting for the electron basic level as well as for the basic light hole one. It is important to mention that the number of peaks expected in Fig. 1 are ten, however the precision used in the calculations does not resolve them properly.

Menendez et al. have performed light scattering experiments in parabolic quantum wells [2]. They found that the energy levels are not equally spaced. For a sample quoted to have $x_B = 0.3$, $d_W = 510$ Å, they reported $E_{01} = 25.2$ meV and $E_{12} = 23.6$ meV with an error of 0.2 meV. They attributed the discrepancy to the fact that the structure consist of a large number of square quantum wells rather than a parabolic graded profile. Moreover, from resonance Raman scattering they found the value $x_B = 0.25$ in disagreement with the value $x_B = 0.3$ deduced from the growth parameters. For the same system parameters, $d_W = 510$ Å and $x_B = 0.3$ ($x_B = 0.25$), we obtain $E_{01} = 22$ meV (21 meV) and $E_{12} = 22$ meV (19 meV). In the case of $x_B = 0.3$ our results are also in closed agreement to the value (22.3 meV) reported by Miller et al. [1]. Shen et al. have studied the energy levels, wave functions and tunability of two coupled PQW's under applied electric field by means of the transfer-matrix method [4]. They report a value of 160 meV (measured from the band edge) for the basic electron level when $d_B = 30$ Å, $d_W = 100$ Å, and well depth of 224 meV, without bias. We obtain for the same system parameters a value of 173 meV.
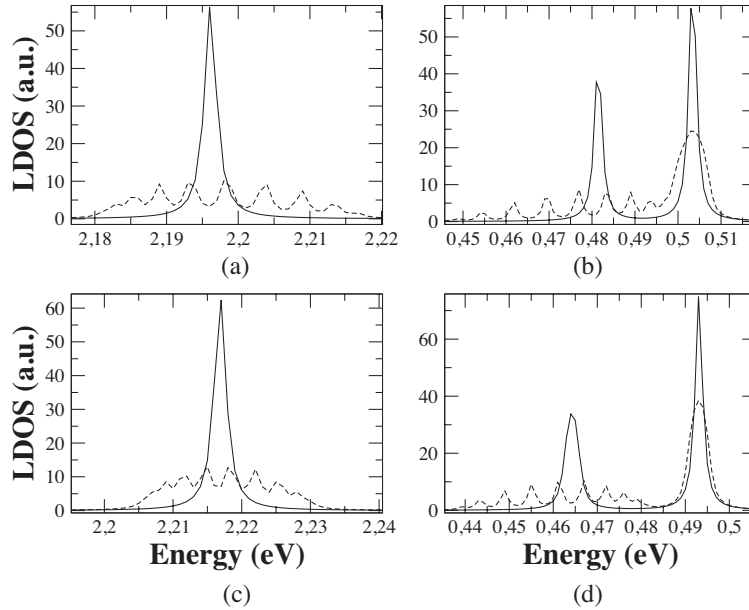
Figure 1. Density of states versus energy of ten period PQWSL's for conduction ((a) and (c)) and valence band ((b) and (d)), for $x_B = 0.21$ ((a) and (b)) and $x_B = 0.30$ ((c) and (d)), well width of 16 ML's and barrier width of 4 ML's. The solid line represents an isolated PQW and the dashed line the PQWSL.

4. CONCLUSION

In summary, we have computed the electronic structure of parabolic $GaAs/Al_xGa_{1-x}As$ superlattices within the spin-dependent sp^3s^* tight-binding model. Clear evidence of the miniband structure formation and the equally spaced energy spectra is found. We also compared our results with the theoretical and experimental data available, obtaining good agreement.

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