Quasi-bound Electronic States in Multiple Delta-doped Quantum Wells

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Abstract— Multiple delta-doped quantum wells of n-type (Si doped $GaAs$) and p-type (Be doped $GaAs$) are studied theoretically looking for quasi-bound electron and hole states. The existence of these states and their strong energy and spatial localizations are demonstrated. The line-width and the mean life time are calculated. The FWHM is less than 10^{-11} eV (10^{-9} eV) and the corresponding mean life time is greater than 10^{-5} s (10^{-7} s) for n- (p-) type wells respectively. A strong spatial localization is observed in both cases.

1. INTRODUCTION

The development of the time-resolved spectroscopy permits the detection of the quasi-bound electronic states in different semiconductor heterostructures [1]. The application of the optical transitions involving quasi-bound states in many semiconductor devices has increased recently [2]. Mean life times of the order of pico-seconds or more are sufficiently large for the design of opto-electronic devices where the quasi-bound states play an important role [3]. There are a lot of theoretical and experimental studies about the above barrier resonances and quasi-bound states in superlattices and multiple quantum wells [4]. There are few investigations of the quasi-bound states in single and isolated multiple quantum wells [5]. The delta-doped quantum wells possess confining potentials of a special type. The discrete part of the energy spectrum of these wells is widely studied [6] and numerous applications in modern semiconductor devices as delta-FET, ALD-FET, etc. are realized [7]. There are very few studies of the continuous part of the electronic spectrum in delta-doped wells [8]. The aim of this work is to demonstrate the promising characteristics of the delta-doped quantum wells to confine quasi-bound states in the conduction and valence band. These states have large mean life times and strong spatial localizations suitable for device applications.

2. MATHEMATICAL METHOD

Isolated multiple delta-doped quantum wells of n-type ($GaAs$ doped with Si) and p-type ($GaAs$ doped with Be) are considered for the usual impurity concentrations ranging the interval between $1 \times 10^{12}\,\text{cm}^{-2}$ and $10^{13}\,\text{cm}^{-2}$. The line-width of the quasi-bound states (FWHM) and the corresponding mean life time (t) are calculated following the methodology and the numerical scheme published recently [5]. The quantum-mechanical treatment is conducted within the framework of the Surface Green Function Matching method (SGFM) in the context of the discrete semi-empirical tight-binding model working in sp^3s^* spin dependent basis [9].

3. RESULTS AND DISCUSSION

3.1. Multiple Delta-doped Quantum Wells of n-type

In the Table 1 the main results for the n-type wells are presented. The number of the quasi-bound electron states and the quantum-mechanical description of the first state (energy, FWHM and mean life time) are given in dependence on the impurity concentration and the barrier height (well depth). The zero of the energy scale is fixed at the bottom of the $GaAs$ conduction band and the energy interval under consideration reaches to 1 eV above the band edge. The number of the quasi-bound states increases from 7 to 21 when the concentration varies from $n_{2D} = 1 \times 10^{12}\,\text{cm}^{-2}$ to $n_{2D} = 10^{13}\,\text{cm}^{-2}$ as consequence of the well depth increase (from 50 meV to 316 meV). When the impurity concentration increases the quasi-bound states move closer to the band edge and move away from the well bottom. The energy changes from 566 meV to 340 meV. This behavior is similar to that of the bound states [10]. A strong energy localization can be observed for all concentrations (the FWHM does not exceed 10^{-11} eV). The mean life times take values greater than 10^{-5} s. The quantum-mechanical characteristics of all quasi-bound states obey similar dependence.

Table 1: *GaAs Si*-doped quantum well. The number of quasi-bound (QB) states, the barrier height (BH), the energy, the full width at half maximum and the mean life time of the first quasi-bound state for different impurity concentrations are given. The zero of the energy is fixed at the bottom of the *GaAs* conduction band. We have look for the quasi-bound states (QB) in the energy interval [0.,1.] eV. The values in parentheses are measured with respect to the bottom of the quantum well.

n_{2D}	1	2	3	4	5	6	7	8	9	10
No.QBS	7	10	12	15	17	18	19	20	21	21
BH *meV*	50	87	121	152	182	210	238	264	290	316
E(QB 1) *meV*	566 (616)	535 (622)	507 (628)	480 (632)	455 (637)	431 (641)	408 (646)	385 (649)	362 (652)	340 (656)
FWHM *eV*	$\leq 10^{-11}$	$\leq 10^{-11}$	$\leq 10^{-11}$	$\leq 10^{-11}$	$\leq 10^{-11}$	$\leq 10^{-11}$	$\leq 10^{-11}$	$\leq 10^{-11}$	$\leq 10^{-11}$	$\leq 10^{-11}$
t, s	$\geq 10^{-5}$	$\geq 10^{-5}$	$\geq 10^{-5}$	$\geq 10^{-5}$	$\geq 10^{-5}$	$\geq 10^{-5}$	$\geq 10^{-5}$	$\geq 10^{-5}$	$\geq 10^{-5}$	$\geq 10^{-5}$

Table 2: *GaAs Be*-doped delta quantum well. The number of quasi-bound (QB) states, the barrier height (BH), the energy, the full width at half maximum and the mean life time of the first quasi-bound state for different impurity concentrations are given. The zero of the energy is fixed at the top of the *GaAs* valence band. We have look for the quasi-bound states (QB) in the energy interval [0.,−1.] eV. The values in parentheses are measured with respect to the bottom of the quantum well.

p_{2D}	1	2	3	4	5	6	7	8	9	10
No.QB S	1	1	1	1	1	1	1	1	1	1
BH *meV*	13	23	31	40	47	55	62	69	76	82
E(QB1) *meV*	−359 (372)	−357 (380)	−355 (386)	−353 (393)	−351 (398)	−350 (405)	−348 (410)	−346 (415)	−345 (421)	−343 (425)
FWHM *eV*	$\leq 10^{-9}$	$\leq 10^{-9}$	$\leq 10^{-9}$	$\leq 10^{-9}$	$\leq 10^{-9}$	$\leq 10^{-9}$	$\leq 10^{-9}$	$\leq 10^{-9}$	$\leq 10^{-9}$	$\leq 10^{-9}$
t, s	$\geq 10^{-7}$	$\geq 10^{-7}$	$\geq 10^{-7}$	$\geq 10^{-7}$	$\geq 10^{-7}$	$\geq 10^{-7}$	$\geq 10^{-7}$	$\geq 10^{-7}$	$\geq 10^{-7}$	$\geq 10^{-7}$

3.2. Multiple Delta-doped Quantum Wells of p-type

The results of the p-type wells are listed in the Table 2 for the same impurity concentrations as in the n-type case. The zero of the energy scale is fixed now at the top of the *GaAs* valence band. The barrier height increases from 13 meV ($p_{2D} = 1\times 10^{12}\,\mathrm{cm}^{-2}$) to 82 meV ($p_{2D} = 10^{13}\,\mathrm{cm}^{-2}$). Only one quasi-bound hole state was found for each concentration in the energy interval of 1 eV above the top of the *GaAs* valence band. The energy of this state approaches the band edge and goes away from the well bottom when the doping concentration increases. The energy values are −359 meV and −340 meV for the lowest and highest concentration respectively. The FWHM parameter maintains no greater than 10^{-9} eV and the mean life time is higher than 10^{-7} s.

3.3. Comparison between the Multiple Delta-doped Wells of n- and p-type

In energy intervals of the same magnitude (1 eV) above the band edges the n-type wells confine 21 quasi-bound states and the p-type wells confine only 1 state. There are two reasons to explain this difference in the capacity to create quasi-bound states. The first reason is that the n-type well is deeper for all concentrations, see Tables 1 and 2. The second one consists in the lower bulk density of states of the valence band comparing with the bulk density of states of the conduction band in the corresponding energy intervals. The electron quasi-bound states are much more localized energetically than the hole states. The FWHM takes values of 10^{-11} eV and 10^{-9} eV respectively for n- and p-type delta well. As a consequence the mean life time is larger in the n-type wells (10^{-5} s) than in the p-type wells (10^{-7} s).

In general, a strong energy localization implies strong spatial localization too. In the Fig. 1 the spectral strengths of the first quasi-bound states for electrons and holes are shown for an impurity concentration of $10^{13}\,\mathrm{cm}^{-2}$. The electron quasi-bound state is much stronger localized spatially than the hole state. The spectral strengths in the wells differ about 5 times and the oscillations outside the wells approximately 20 times.

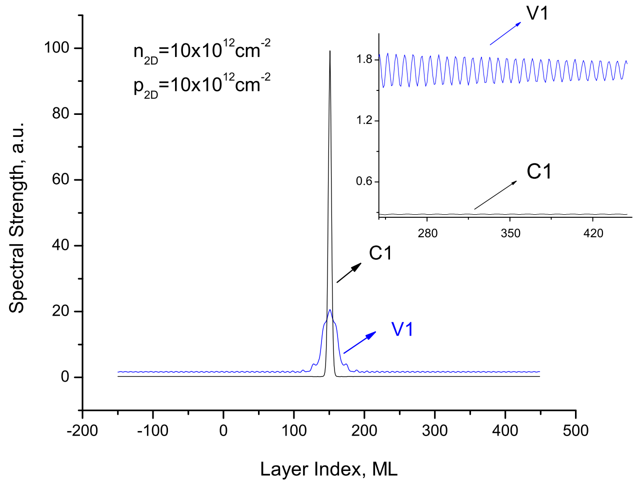

Figure 1: Spectral strengths of the first quasi-bound states for electrons and holes for an impurity concentration of $10^{13}\,\mathrm{cm}^{-2}$.

The quasi-bound states are well separated (see the Tables) which is an important advantage of the delta-doped wells comparing with the rectangular quantum wells [5].

4. CONCLUSION

The isolated multiple delta-doped quantum wells confine strongly quasi-bound electron and hole states having good energy separation. The mean life times and the spatial localizations of these states permit their experimental detection. Some device applications are quite possible.

REFERENCES

1. Colocci, M., J. Martinez-Pastor, and M. Gurioli, "Above-barrier resonant transitions in $Al_xGa_{1-x}As/AlAs/GaAs$ heterostructures," *Phys. Rev. B*, Vol. 48, No. 11, 8089–8094, 1993.
2. Levy, M., R. Kapon, A. Sa'ar, R. Beserman, V. Thierry-Mieg, and R. Planel, "Modulated resonant Raman and photoluminescence spectroscopy of Bragg confined asymmetric coupled quantum wells," *Physica E*, Vol. 7, No. 1–2, 245–249, 2000.
3. Sung, B., H. C. Chui, E. L. Martinet, and J. S. Harris, Jr., "Control of quasi-bound states by electron Bragg mirrors in $GaAs/Al_{0.3}Ga_{0.7}As$ quantum wells," *Appl. Phys. Lett.*, Vol. 68, No. 19, 2720–2722, 1996.
4. Satanin, A. M. and Y. S. Joe, "Fano interference and resonances in open systems," *Phys. Rev. B*, Vol. 71, No. 20, 205417, 2005.
5. Vlaev, S. J. and V. M. González Robles, "Mean lifetimes of quasi-bound electronic states in single rectangular quantum wells," *Phys. Stat. Sol. (C)*, Vol. 2, No. 10, 3653–3656, 2005.
6. Gaggero-Sager, L. M. and R. Pérez-Alvarez, "Self-consistent energy levels in p-type delta-doped quantum wells in GaAs," *J. Appl. Phys.*, Vol. 79, No. 6, 3351–3353, 1996.
7. Martínez-Orozco, J. C., L. M. Gaggero-Sager, and S. J. Vlaev, "A simple model for the differential capacitance profile in the atomic layer doped field effect transistor (ALD-FET) in GaAs," *Materials Science and Engineering B*, Vol. 84, No. 3, 155–158, 2001.
8. Vlaev, S. J., I. Rodriguez-Vargas, and L. M. Gaggero-Sager, "Resonant states in n-type δ-doped GaAs quantum wells," *Phys. Stat. Sol. (C)*, Vol. 2, No. 10, 3649–3652, 2005.
9. Vlaev, S., V. R. Velasco, and F. García-Moliner, "Electronic states in graded-composition heterostructures," *Phys. Rev. B*, Vol. 49, No. 16, 11222–11229, 1994.
10. Vlaev, S. J. and L. M. Gaggero-Sager, "Thomas-Fermi approximation in a tight-binding calculation of δ-doped quantum wells in GaAs," *Phys. Rev. B*, Vol. 58, No. 3, 1142–1145, 1998.