Quantum wells delta-doped to the center with background doping in barriers

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1. Introduction

As is known during the heterostructure growth the background impurity is introduced in their content. The ionization of such an impurity can affect essentially the optical and electrophysical properties of the heterostructure and the entire device. Our work is devoted to the theoretical study of the influence of the background impurity to the redistribution of carriers within QW and consequent changes of energy spectrum and impurity ionization energy of the n-type $Si_{0.8}Ge_{0.2}/Si/Si_{0.8}Ge_{0.2}$ QWs delta-doped by Phosphorus in the center and in the edge of the well. Calculations were performed for the temperatures T=4, 77, 300K. The background impurity concentration N_b has been taken as 10^{15} cm^{-3}, 10^{16} cm^{-3}, и 10^{17} cm^{-3}. It should be noted that even at low temperature there are free electrons inside the QW (and positive ions at the barriers). With increasing of temperature is switched ionization of the impurity delta-layer. As a result we observe the "competition" of two sources of free carriers: delta layer inside the QW and background impurity at barriers. Thus we have a distortion of the energy profile of QW with a new set of space-quantized energy levels and accordingly with a new impurity binding energy. Therefore the ***aim of the work*** is to present our results of the investigation of this phenomenon.

2. Comments on the chosen object

We study $Si_{0.8}Ge_{0.2}/Si/Si_{0.8}Ge_{0.2}$ QW structures with infinitely wide barriers in both sides. Phosphorus δ-doping layer is positioned inside the well near either center or edge of QW. Calculations were performed for width of QW (L=20nm), concentration of the impurity delta-layer (N=1.2x10^{12} cm^{-2}), concentrations of background impurity (N_b=10^{17}, 10^{16}, 10^{15} cm^{-3}) and temperatures (T=4, 77, 300K).

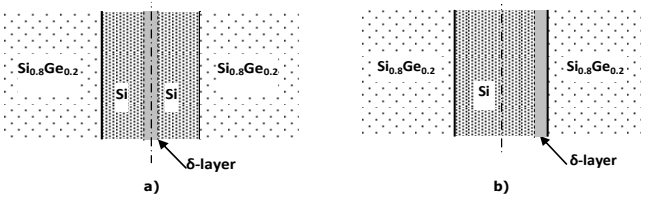


FIG.1 $Si_{0.8}Ge_{0.2}/Si/Si_{0.8}Ge_{0.2}$ QW structure, a) – center-doped QW, b) – edge-doped QW.

3. Method

Our calculations are performed in the effective mass approximation. To simplify the Hamiltonian of the problem, some assumptions have been made. They are single impurity approach, neglecting exchange and correlation interaction and others, more details described in the work [3]. Positions of the energy subbands as well as IBE for different temperatures was found from self-consistent solution of Schrodinger, Poisson, and electroneutrality equations. All calculations were carried out iteratively. At each stage the Hartree potential formed by the ionized impurity delta layer and electrons in the QW was allowed for within the self-consistent solution of the equations of electrical neutrality and Poisson.

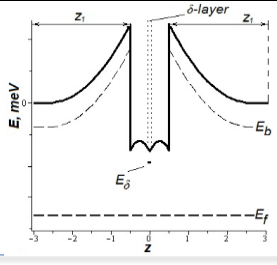
In the first step to calculate the Hartree potential we used the value of the ionization energy of delta-layer impurity calculated for QW without the background impurity in the work [2]. Then the Schrodinger equation with the Hamiltonian including Hartree's potential was solved to find the size-quantization levels and wave functions of the carriers in the QW. Values of energies of the subbands and wave functions were used to calculate the impurity ionization energy by the Vinter method [1]. The obtained value of the binding energy and the rate of ionization of the background impurity were used to refine the Hartree potential, position of size-quantization levels and wave functions during the next iteration. Calculations finished when the ionization energy values obtained for the successive iterations do not differ by more than 0.1 meV.

4. Results

TABLE 1. Positions of Fermi level (**E_f, meV**), impurity binding energy of Δ-layer donors (**E_δ, meV**) of $Si_{0.8}Ge_{0.2}/Si/Si_{0.8}Ge_{0.2}$ QW structures. **N_{QW} (cm^{-3})** – concentration of free electrons inside the QW. Width of QW (L=20nm), concentration of the impurity delta-layer (N=1.2*10^{12} cm^{-2}), concentrations of background impurity (N_b=10^{17}, 10^{16}, 10^{15} cm^{-3}) and temperatures (T=4, 77, 300K). Zero of energy is at the bottom of the conduction band for z→±∞ (shown at the fig. 2). **E_f, E_δ** counted from the first space quantized energy level.

N_b =10^{17}cm^{-3}	(Center-Doped QWs)			(Edge-Doped QWs)		
	T = 4 K	T = 77 K	T = 300 K	T = 4 K	T = 77 K	T = 300 K
N_{QW}, cm^{-2}	8.7*10^{11}	9.5*10^{11}	1.5*10^{12}	8.7*10^{11}	9.0*10^{11}	1.3*10^{12}
E_f, meV	-19.0	-34.0	-146.1	-19.0	-34.0	-146.1
E_δ, meV	**-17.8**	**-19.5**	**-32.4**	**-27.2**	**-27.5**	**-32.4**
N_b =10^{16}cm^{-3}	(Center-Doped QWs)			(Edge-Doped QWs)		
	T = 4 K	T = 77 K	T = 300 K	T = 4 K	T = 77 K	T = 300 K
N_{QW}, cm^{-2}	2.9*10^{11}	3.6*10^{11}	9.9*10^{11}	2.9*10^{11}	3.7*10^{11}	8.6*10^{11}
E_f, meV	-19.4	-43.3	-205.0	-19.4	-43.3	-205.0
E_δ, meV	**-26.9**	**-27.8**	**-33.4**	**-21.5**	**-24.2**	**-31.7**
N_b =10^{15}cm^{-3}	(Center-Doped QWs)			(Edge-Doped QWs)		
	T = 4 K	T = 77 K	T = 300 K	T = 4 K	T = 77 K	T = 300 K
N_{QW}, cm^{-2}	9.4*10^{10}	1.8*10^{11}	8.4*10^{11}	9.4*10^{10}	2.2*10^{11}	7.5*10^{11}
E_f, meV	-19.8	-55.3	-264.5	-19.8	-55.3	-264.5
E_δ, meV	**-28.5**	**-29.4**	**-33.7**	**-18.5**	**-23.6**	**-31.6**

FIG. 2 Schematic view of the center doped QW with the background impurity at the barriers.



At the fig. 2 is shown distortion of the shape of the conductivity band bottom of the QW, due to the temperature ionization of the impurity delta-layer inside the well and ionization of the background impurity at the barriers. This sketch allows to understand our choice of zero of energy of the next figures, namely, zero of energy corresponds to the bottom of the conduction band, when z→±∞.

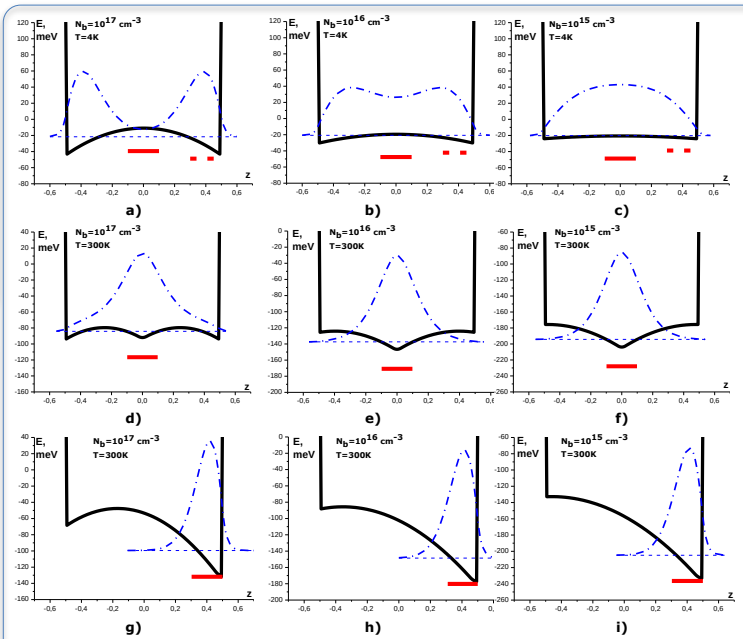


FIG. 3 Energy profile – solid black lines, 1-st space quantization levels and their wave functions dashed and dot-dashed blue lines, respectively, ground impurity states–solid red lines (a-c – center- and edge-doped QWs; ground impurity states for center-doped QWs – solid red lines, ground impurity states for edge-doped QWs – dashed red lines) for $Si_{0.8}Ge_{0.2}/Si$ QW, L = 20 nm, T=4K (a-c) and 300K (d-i), delta-doped at the center (a-f) and at the edge of the QW (a-c and g-i).

TABLE 2. Positions of first five space quantized energy levels (**E_i, meV**), $Si_{0.8}Ge_{0.2}/Si/Si_{0.8}Ge_{0.2}$ QW structures. Zero of energy is at the bottom of the conduction band for z→±∞ (shown at the fig. 2).

N_b =10^{17}cm^{-3}	(Center-Doped QWs)			(Edge-Doped QWs)		
	T = 4 K	T = 77 K	T = 300 K	T = 4 K	T = 77 K	T = 300 K
E_1, meV	-21.7	-28.3	-84.2	-21.7	-28.9	-99.5
E_2, meV	-21.6	-28.2	-78.2	-21.6	-27.1	-72.1
E_3, meV	-10.4	-18.1	-75.8	-10.4	-16.5	-54.2
E_4, meV	-6.3	-13.5	-69.0	-6.3	-12.5	-48.9
E_5, meV	1.8	-5.6	-60.8	1.8	-4.3	-42.5
N_b =10^{16}cm^{-3}	(Center-Doped QWs)			(Edge-Doped QWs)		
	T = 4 K	T = 77 K	T = 300 K	T = 4 K	T = 77 K	T = 300 K
E_1, meV	-20.8	-30.4	-137.4	-20.8	-32.5	-148.5
E_2, meV	-19.6	-28.8	-126.1	-19.6	-26.8	-122.7
E_3, meV	-14.5	-24.2	-120.4	-14.5	-23.4	-104.4
E_4, meV	-8.0	-17.5	-114.0	-8.0	-16.9	-91.2
E_5, meV	0.4	-9.1	-106.1	0.4	-8.6	-82.7
N_b =10^{15}cm^{-3}	(Center-Doped QWs)			(Edge-Doped QWs)		
	T = 4 K	T = 77 K	T = 300 K	T = 4 K	T = 77 K	T = 300 K
E_1, meV	-20.3	-38.4	-194.3	-20.3	-41.6	-204.8
E_2, meV	-18.0	-35.3	-181.9	-18.0	-34.3	-178.9
E_3, meV	-13.3	-30.9	-175.0	-13.3	-30.0	-160.1
E_4, meV	-6.7	-24.2	-168.1	-6.7	-23.8	-145.7
E_5, meV	1.9	-15.7	-160.1	1.9	-15.5	-135.0

5. Conclusions

1. The obtained results for the low concentration of the background impurity confirmed the data of the work [2] as to general behavior of the impurity binding energies with temperature. Namely, the temperature increase from 4 to 300 K does not influence it much for the center-doped impurity delta-layer and that influence is quite a big for the edge-doped QW.

2. The dependencies of impurity binding energy on impurity concentration in barriers are different for edge-, and center-doped layers. For the first one it decreases with concentration of background impurities and for the second case – it increases.
This effect is more developed at the case of low temperature (pic. 3 a-c). With decreasing of the concentration of the background impurity, the localization of free electrons at the first space quantization level shifts to the center of the QW (see changes of the shape of the correspond wave function). Thus at the case of the center-delta-doping the Coulomb repulsion between free electrons and electrons in the impurity increases. Consequently, the impurity binding energy is increase. At the case of the edge-delta-doping the Coulomb repulsion decreases. Consequently, the impurity binding energy is decrease.

3. As shown at the table 2, with changing of the temperature and of the concentration of the background impurity, the difference between first quantization levels changes too. This effect is reflected on optical properties of heterostructure and can be used at the design of optical devises on the base of delta-doped QWs.

6. Literature cited

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