Shallow impurities in delta-doped Si quantum well under a transversal electric field

Demediuk, R.[1], **Tulupenko, V.**[1,4], **Akimov, V.**[1,2], **Tiutiunnyk, A.**[3],
Duque, C.[1,4], **Sushchenko, D.**[1], **Fomina, O.**[1], **Laroze, D.**[3]
[1] *Physics Department, Donbas State Engineering Academy, Academichna str., 72, Kramatorsk-84313, Donetsk reg., Ukraine.*
E-mail: demediuk.roman@gmail.com
[2] *Facultad de Ciencias Basicas, Grupo de Materia Condensada-UdeA, Universidad de Medellín, Medellín, Colombia.*
[3] *Instituto de Alta Investigación, CEDENNA, Universidad de Tarapacá, Arica, Chile.*
[4] *Grupo de Materia Condensada-UdeA, Universidad de Antioquia, Medellin, Colombia.*

INTRODUCTION

Using optical transitions between size-quantized subbands in quantum wells (QWs) implies the frequency range starting from near infrared and below, for the most common semiconductor materials. Currently, from the engineering point of view, the most attractive (and most problematic) is the TeraHertz (THz) range, which is on the border between optics (infrared, IR) and electronics (microwave).

An impurity delta-layer positioned inside the quantum well may be used as a factor allowing control over the energies of the intersubband optical transitions or, in other words, it opens possibilities for the creation of new types of tunable by an external longitudinal electric field THz optical device. The **idea** is the following. Initially, the impurity is not ionized (implying low temperature) and the potential profile of the QW has, for example, a classic rectangular shape. When an electric field in the plane of the QW is applied, the electric current is formed, the impurity is ionized by an impact mechanism and the charge redistribution in the direction perpendicular to the QW plane distorts the potential profile. The distorted profile changes (normally increases) the energy distances between the size-quantized subbands so that the energy of the peak optical response grows as well.

Aims of this work are the following. First, to show the possibility of the tuning of energy distances between first space quantized levels by both the external electric field transversally applied to the QW and the temperature. Second, to compare the cases of delta-doping at the center and at the edge of QWs in this regard.

METHODS

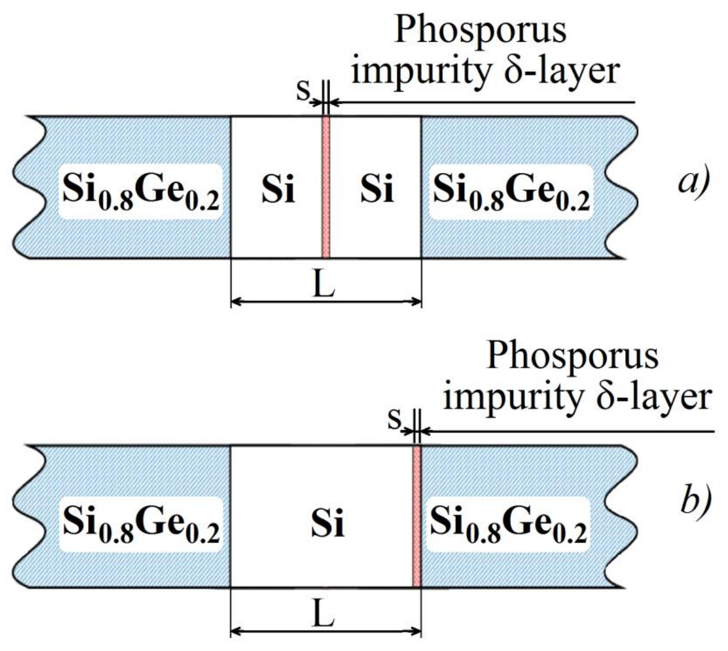

Fig. 1. Schematic representation of the heterostructure under study. Center-doped QW – a); edge-doped QW – b).

The object of investigation is a doped rectangular $Si_{0.8}Ge_{0.2}$/Si/ $Si_{0.8}Ge_{0.2}$ QW with the shallow donor impurity delta-level positioned within the Si layer at the center Fig.1 a) or at the edge Fig.1 b). The well width is L = 20 nm. The delta-layer width is taken as s = 1 nm. The sheet concentration of the donors in the delta-layer was taken as 1.2 x 10^{12} cm^{-2}. Calculation was carry out for two temperatures (degree of ionization of the impurity delta-layer): 4K – without ionization and 300 – the ionization is about 70%.

The presented results were obtained by a self-consistent solution of the following. (i) one-dimensional static Schrodinger equation to obtain bound in z-direction electronic states (edges of size-quantized subbands) and corresponding wave functions; (ii) electroneutrality equation implying equilibrium Fermi-Dirac statistics to obtain the Fermi level of the well; (iii) Poisson equation to obtain the Hartree potential *φ(z)* due to the redistribution of positive charges of ionized impurities and negative charges of electrons; (iv) obtaining impurity binding energy with a method first proposed in [1].

The Hamiltonian for the Schrodinger equation is $H_0 = -\frac{\hbar^2}{2m_\perp}\frac{\partial^2}{\partial z^2} + V(z) + eEz + e\varphi(z)$, where e is unit charge and $m_\perp$ is the electron effective mass in the *z*-direction, $V(z)$ – the undisturbed well potential profile, E – the electric field strength, $\varphi(z)$ – the Hartree potential, was obtained from the Poisson equation: $\frac{\partial^2\varphi}{\partial z^2} = \frac{e}{\varepsilon\varepsilon_0}N(z)$, with $N(z)$ being 3-dimensional concentration of charge consisting of positive ionized shallow donor centers N_D and negative electrons in the subbands of quantum well N_e: $N(z) = N_D(z) - N_e(z)$. Ionized donors are concentrated in the delta-layer and their concentration is calculated within quasi-Fermi statistics, for the center-doped case as $N_D(z) = \begin{cases} \frac{n_\delta/s}{1+2\exp(\frac{E_F-E_\delta}{kT})}, & |z| < \frac{s}{2} \\ 0, & |z| \geq \frac{s}{2} \end{cases}$. Electron concentration distribution along z is obtained according to the same statistics as: $N_e = \frac{m_\parallel kT}{\pi\hbar^2}\sum_j \ln\left(1 + exp\frac{E_F - E_j}{kT}\right)\left|\xi_j(z)\right|^2$, $m_\parallel$ – being an effective mass of the well material in plane of quantum well, E_j and $\xi_j(z)$ are eigenvalues and normalized eigenfunctions of the Hamiltonian.

RESULTS

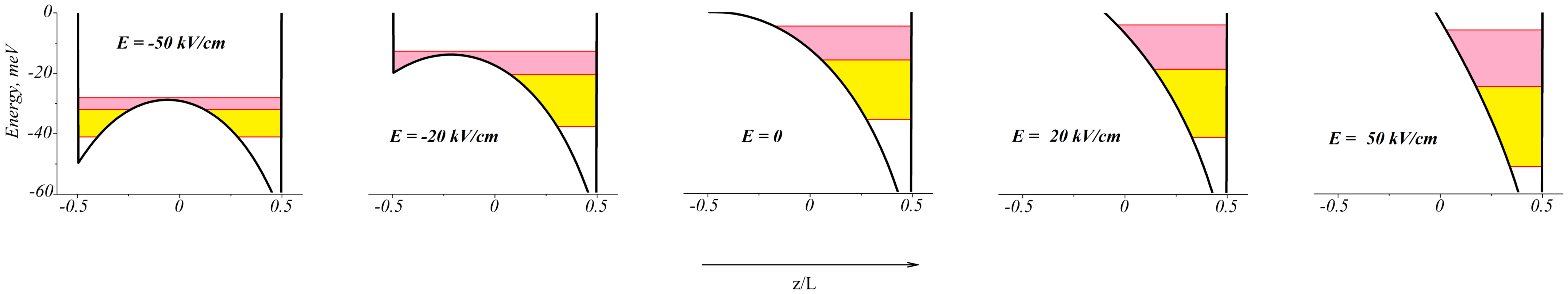

Fig. 2. Energy profile (black line) of the 20 nm wide quantum well with impurity delta-layer in the edge in transverse electric field *E*. Red lines are first three space-quantized energy levels. The temperature is T=300K. All the graphs have the same energy scale factor. The opposite direction of electric field with respect to z-direction marked as “-”.

Table 1. Energy distances between first two space-quantized levels ΔE_{21} (meV) of the 20 nm wide QW, with impurity delta-layer in the edge or in the center, in transverse electric field E.

E (kV/cm)		-100	-50	-20	-10	0	10	20	50	100
4 K	Edge- or center-doping	28.2	17.8	9.7	6.1	2.8	6.1	9.7	17.8	28.2
300 K	Edge-doping	15.8	9.1	17.2	18.6	19.7	21.2	22.6	26.6	33.6
	Center-doping	13.0	4.8	8.8	10.2	11.1	10.2	8.1	4.8	13.0

CONCLUSIONS

- The grade of ionization of impurity delta-level affects significantly the energy distance between the first two quantized levels for all configurations under study that permits tuning the energies of intersubband optical transitions with a lateral electric field.
- The transverse electric field also has a strong influence on the tuning effect that can not be neglected and is the most pronounced in case of edge delta-doping.
- For the temperature T = 4K, the direction of an electric field does not affect the energy distances between space-quantized levels for both positions of the doping (Table 1, T=4K).
- It is also correct for the elevated temperature for the case of a center-doping (Table 1, T=300K, center-doping). The situation is different for the case of an edge-doping. The data of the Table 1 shows the increase of the energy distance between 2 and 1 space-quantized levels when the strength of the electric field grows from about -50 kV/cm (yellow region in graphs of the Figure 2).
- The pink band width dynamics in Fig. 2 shows the growth of ΔE_{32} – energy distance between 3 and 2 space-quantized levels. But to a lesser degree in comparison with ΔE_{21} .

REFERENCES

[1] Vinter B 1982 *Phys. Rev. B* **26** 6808.