ФІЗИКА І ХІМІЯ ТВЕРДОГО ТІЛА
Т. 14, № 1 (2013) С. 213-217

PHYSICS AND CHEMISTRY OF SOLID STATE
V. 14, № 1 (2013) P. 213-217

PACS: 73.63.Kv, 73.20.At

ISSN 1729-4428

V.V. Kuryliuk, O.A. Korotchenkov, A.B. Nadtochiy

Strain Relaxation in Si/Ge Heterostructures with Quantum Dots

Faculty of Physics, Taras Shevchenko Kyiv National University,
Volodymyrska Str. 64, Kyiv, 01601, E-mail: kuryluk@univ.kiev.ua

The influence of a thin SiO_2 layer, placed between the Si substrate and Ge quantum dot, on the strain relaxation inside the substrate is computationally investigated employing FEM techniques. Concomitant modifications of the band structure near the interface are also analyzed. Experimental surface distributions of the surface photovoltage signal give a general framework of a spatial distribution of the photogenerated electrons and holes near the interface relevant to the generation of capturing potential caused by the dots.

Key words: quantum dot, strain, relaxation, photovoltage.

Стаття поступила до редакції 25.10.2012; прийнята до друку 15.12.2012.

Introduction

SiGe heterostructures with quantum dots (QDs) Ge offer advantage of strain relaxation in the strained silicon substrate, which originates from the difference in the lattice parameters of silicon and germanium (5,43 and 5,65 Å, respectively) [1, 2]. In addition, the strain relaxation processes allow remarkable changes in the confinement-potential for charged carriers, forming potential minima for electrons in Si substrate and changing the energy spectrum of holes in QDs [3].

This work is devoted to theoretical investigation of the influence of a thin SiO_2 layer, placed between the Si substrate and Ge QD, on the strain relaxation inside the substrate. Appropriate modifications of the band structure near the interface are also analyzed. Computations are made employing FEM technique and computational details are given elsewhere [3]. We shall also give the experimentally taken surface distributions of the surface photovoltage (SPV) signal, which is sensitive to the value of a spatial distribution of the photogenerated electrons and holes near the interface.

I. Theoretical and experimental procedure

Our calculations of the elastic deformation around the QD are limited to consideration of a cell that contains a single dot in the form of rectangular pyramid, placed on the substrate with $L_x \times L_y = 60 \times 60$ nm in cross-section and $L_z = 20$ nm in thickness (Fig. 1). The dot height h and the base length a are equal to 3 and 24 nm, respectively. We shall consider two substrate types, one of which consists of a silicon plate, and the other one of a thin ($d = 2$ nm)

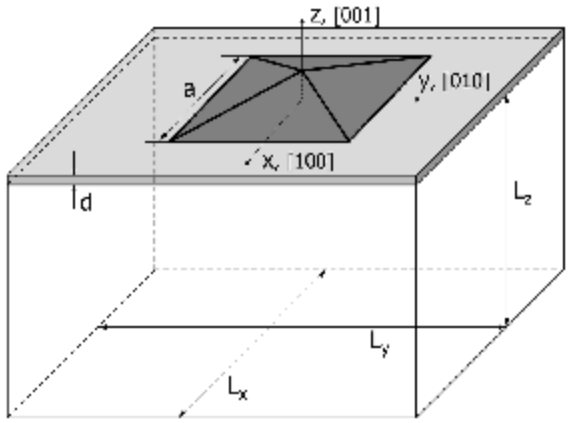

Fig. 1. Geometry of the unit cell used for the finite element calculations.

SiO_2 oxide layer mounted on the Si plate. The origin of the coordinate system coincides with the pyramid base center, and the *x*-, *y*- and *z*-axis are directed along the crystallographic directions [100], [010] and [001], respectively.

SPV transients are measured in the capacitor arrangement [4], and details of our setup are given elsewhere [5]. The scanning SPV apparatus based on the AC-SPV technique [6] and utilizing a "flying spot" arrangement [7] is used for obtaining SPV decays and spatially-resolved SPV maps. This technique is capable of providing wafer maps of both the photovoltage magnitude and carrier lifetime with a 100-μm spatial resolution. The transients were taken using a pump pulse generated by a red laser diode light (LED). The LED beam was focused on the sample surface to a spot smaller than 100 μm thus providing the above resolution.

The LED was controlled by the external bias in the form of square-function pulse. The LED pulse rise and fall times were smaller and the pulse sequence was greater than the SPV decay time. The measuring circuit was carefully screened to ensure the experimental system was not susceptible to electronic pickups or ground loop effects.

II. Results and discussion

The standard elasticity problem is solved that relates the mechanical stress (*T*) and strain (*S*) tensor components in the following form:

$$T_i(\mathbf{r}) = C_{ij}(\mathbf{r}) S_j(\mathbf{r}), \quad i, j \in [xx, yy, zz, yz, xz, xy] \qquad (1)$$

where $C_{ij}(\mathbf{r})$ is the elastic module tensor, $S_i(\mathbf{r}) = \varepsilon_i(\mathbf{r}) - \varepsilon_{0i}(\mathbf{r})$ is the strain tensor, $\varepsilon_i(\mathbf{r})$ is the total strain and $\varepsilon_{0i}(\mathbf{r})$ is the initial strain due to a lattice mismatch between Si and Ge:

$$e_{0i}(\mathbf{r}) = \begin{cases} \left[e_{0xx}, e_{0yy}, e_{0zz}, 0, 0, 0\right]^t & in\ QD-region \\ \left[0,0,0,0,0,0\right]^t, & elsewhere \end{cases}, \qquad (2)$$

Since the material substrate, oxide layer and QDs are characterized by different elastic modules C_{ij}, the corresponding matrix components in Eq. (1) depend upon coordinates. Accounting for the relationship between mechanical deformation and components uk (k = x, y, z) of the elastic displacement vector,

$$e_i(\mathbf{r}) = \nabla_S u_k(\mathbf{r}), \qquad (3)$$

Eq. (1) becomes

$$T_i(\mathbf{r}) = C_{ij}(\mathbf{r})\left(\nabla_S u_k(\mathbf{r}) - e_{0j}(\mathbf{r})\right), \qquad (4)$$

Taking use of an infinite periodic cell structure, the periodicity boundary conditions are satisfied by equating the normal components of the $\mathbf{u}(\mathbf{r})$ vector in the opposite x-and y- faces of the substrate to zero:

$$\begin{aligned} u_x\left(-\frac{L_x}{2}, y, z\right) &= u_x\left(\frac{L_x}{2}, y, z\right) = 0 \\ u_y\left(x, -\frac{L_y}{2}, z\right) &= u_y\left(x, \frac{L_y}{2}, z\right) = 0 \end{aligned}, \qquad (5)$$

The bottom plane of the substrate is considered to be rigid:

$$u_x(x, y, -L_z) = u_y(x, y, -L_z) = u_z(x, y, -L_z) = 0, \qquad (6)$$

In addition, all components of the elastic displacement vector $\mathbf{u}(\mathbf{r})$ are continuous across the substrate-QD boundary:

$$u_i(x, y, 0)\big|_{substrate} = u_i(x, y, 0)\big|_{QD}, \qquad (7)$$

and on the substrate surface and lateral sides of a pyramid the mechanical strain is presumed to be zero (free surfaces):

$$T_{ij} n_j = 0, \qquad (8)$$

The solutions of Eq. (4) with boundary conditions (5) - (8) are the spatial distributions of the $u_i(\mathbf{r})$ components of the elastic displacement vector. Using Eq. (3) and the $u_i(\mathbf{r})$ components, we get the strain $S_i(\mathbf{r})$ distributions.

It is known that there are two strain tensor components that can affect the band structure. First, hydrostatic strain $e_h(\mathbf{r}) = S_{xx}(\mathbf{r}) + S_{yy}(\mathbf{r}) + S_{zz}(\mathbf{r})$, comes from the material's volume change ΔV/V and leads to the conduction and valence band edge shifts by:

$$\Delta E_c(\mathbf{r}) = a_c e_h(\mathbf{r}), \qquad (9)$$

$$\Delta E_v(\mathbf{r}) = a_v e_h(\mathbf{r}), \qquad (10)$$

where a_c and a_v are the hydrostatic deformation potentials for the conduction and valence bands, respectively.

The second component, biaxial strain $e_b(\mathbf{r}) = 2S_{zz}(\mathbf{r}) - S_{xx}(\mathbf{r}) - S_{yy}(\mathbf{r})$, leads to the level splitting in the degenerate bands. For a triply degenerate valence band:

$$\Delta E_{lh}(\mathbf{r}) = -\frac{\Delta_0}{6} + \frac{dE(\mathbf{r})}{2} + \frac{\sqrt{4\Delta_0^2 + 4\Delta_0 dE(\mathbf{r}) + 9dE^2(\mathbf{r})}}{4}, \qquad (11)$$

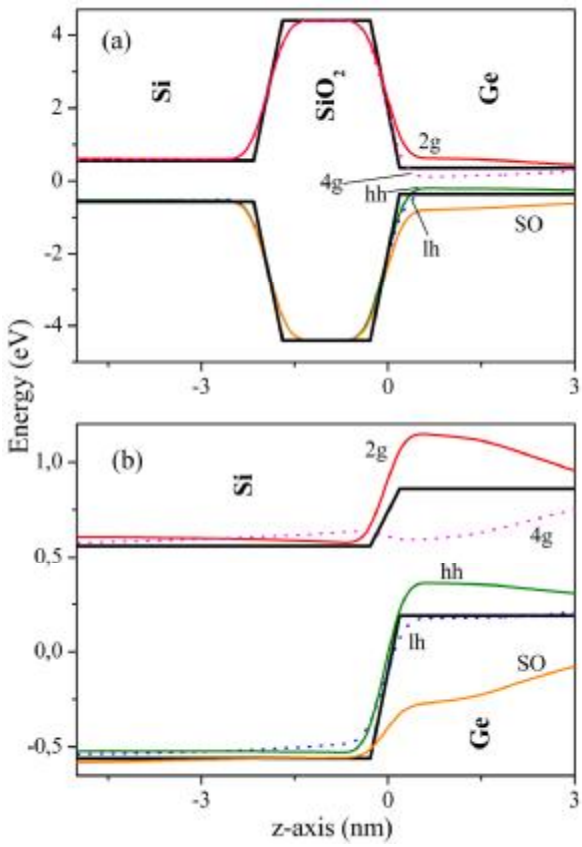

Fig. 2. Conduction and valence band edges inside the Si-SiO_2-Ge (*a*) and Si-Ge (b) structures. $z > 0$ corresponds to Ge QD, $z = 0$ – Si surface in (*b*) and 2-nm thick SiO_2 layer in (a).

$$\Delta E_{hh}(\mathbf{r}) = \frac{\Delta_0}{3} - \frac{dE(\mathbf{r})}{2}, \quad (12)$$

$$\Delta E_{SO}(\mathbf{r}) = -\frac{\Delta_0}{6} + \frac{dE(\mathbf{r})}{4} - \frac{\sqrt{4\Delta_0^2 + 4\Delta_0 dE(\mathbf{r}) + 9dE^2(\mathbf{r})}}{4}, \quad (13)$$

where $\Delta E_{lh}(\mathbf{r})$, $\Delta E_{hh}(\mathbf{r})$, $\Delta E_{SO}(\mathbf{r})$ are the shifts of the levels of light, heavy holes and spin-orbit splitting, respectively, Δ_0 is the spin-orbit splitting constant. For $dE(\mathbf{r})$, we can equate:

$$dE(\mathbf{r}) = b_v e_b(\mathbf{r}), \quad \text{for [001] direction,} \quad (14)$$

$$dE(\mathbf{r}) = \frac{b_{v1}}{\sqrt{3}} e_b(\mathbf{r}), \quad \text{for [111] direction,} \quad (15)$$

where b_v and b_{v1} are the deformation potential constants for the valence band. A uniform deformation in the [111] direction does not affect the structure of the conduction band in Si and Ge, whereas in the [001] direction it produces the splitting of the 6-fold degenerate band into the 4-fold degenerate band (4g) with the energy minimum in the (001) plane, and the 2-fold degenerate band (2g) with the energy minimum normally to the (001):

$$\Delta E_c^{2g}(\mathbf{r}) = \frac{b_c e_b(\mathbf{r})}{3}, \quad (16)$$

$$\Delta E_c^{4g}(\mathbf{r}) = -\frac{b_c e_b(\mathbf{r})}{6}, \quad (17)$$

where b_c is the deformation potential constant for the

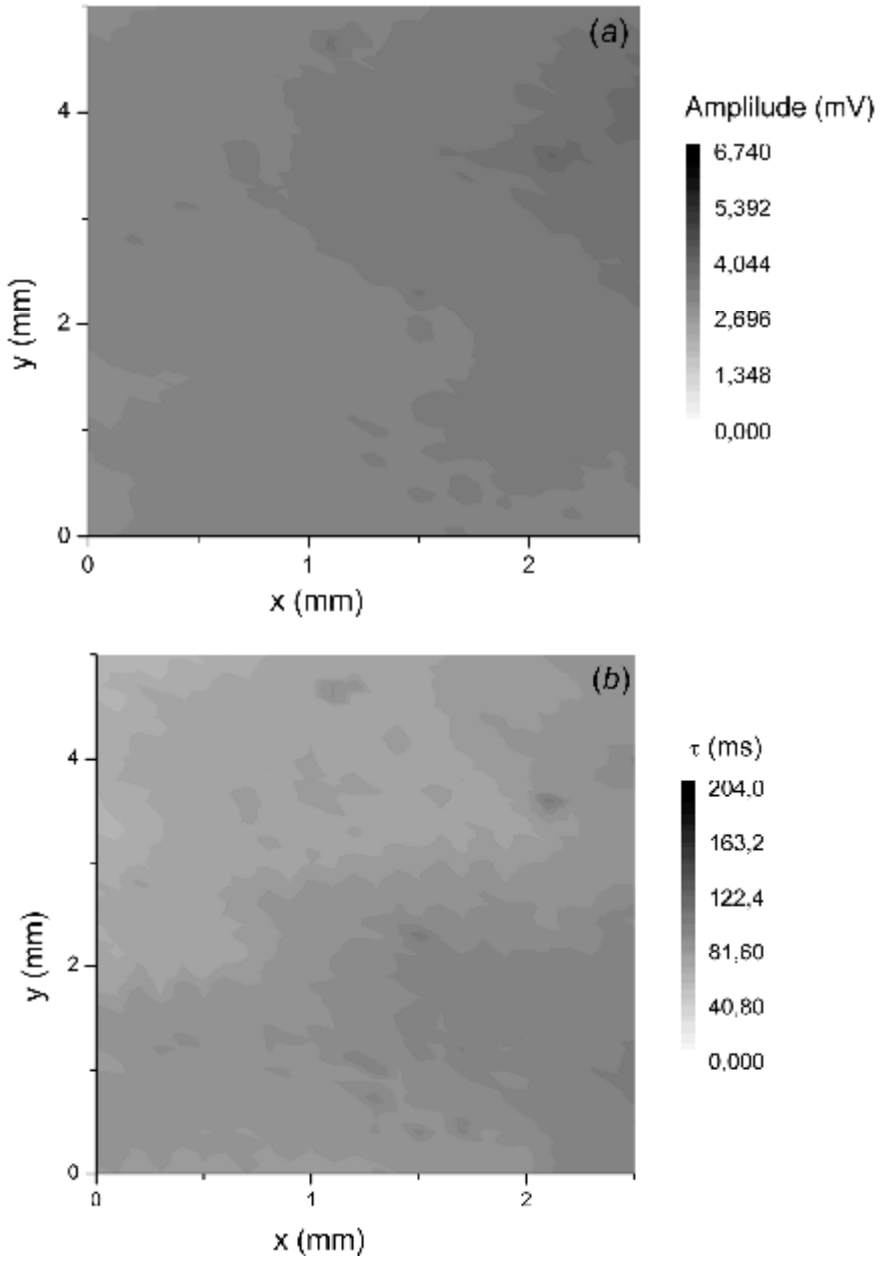

Fig. 3. Spatially resolved SPV amplitude U_0 (*a*) and decay time t (*b*) observed in Si substrate the Si-SiO_2-Ge sample.

conduction band.

The calculation results are given in Fig. 2. It is seen that, in Si-Ge II-type heterostructures, the strain relaxation leads to a low-energy shift of the 2g-conduction band with respect to the 4g-band. Moreover, due to non-uniform strain distribution in the heterostructure, the 2g-energy band edge position also becomes non-uniform. As seen in Fig. 2(b), energy minimum of the 2*g*-band is near the top of the Ge pyramid dot, where the strain reaches its maximum value. Another consequence of the strain effects is the splitting of the energy levels of light and heavy holes in the valence band. As seen in Fig. 1, the energy minima are inside the Ge pyramid.

The inclusion of a thin oxide layer between Si and Ge imposes additional features of strain relaxation in comparison with the Si-Ge heterostructure. In particular, insertion of a SiO_2 oxide layer forces to change the pyramid shape of the dot (in Si-Ge heterostructure) into the semisphere shape in Si-SiO_2-Ge heterostructure, which is accompanied by the dot density increase. Furthermore, the oxide layer offers additional channels for the strain relaxation in SiGe heterostructures.

Taken together, these facts would remarkably affect the strain relaxation in Si-SiO_2-Ge system in comparison with the Si-Ge heterostructure, thus affecting the band structure modification as exemplified in Fig. 2(*a*). Most interestingly, the Si-Ge II-type heterostructure is seemingly transferred into the I-type heterostructure in Si-SiO_2-Ge due to strain relaxation features imposed by a SiO_2 oxide layer. Obviously, further work is needed to confirm this striking result of the simulations.

In this work, we only observe the difference in the photovoltaic performance of a Si substrate and a Si-SiO_2-

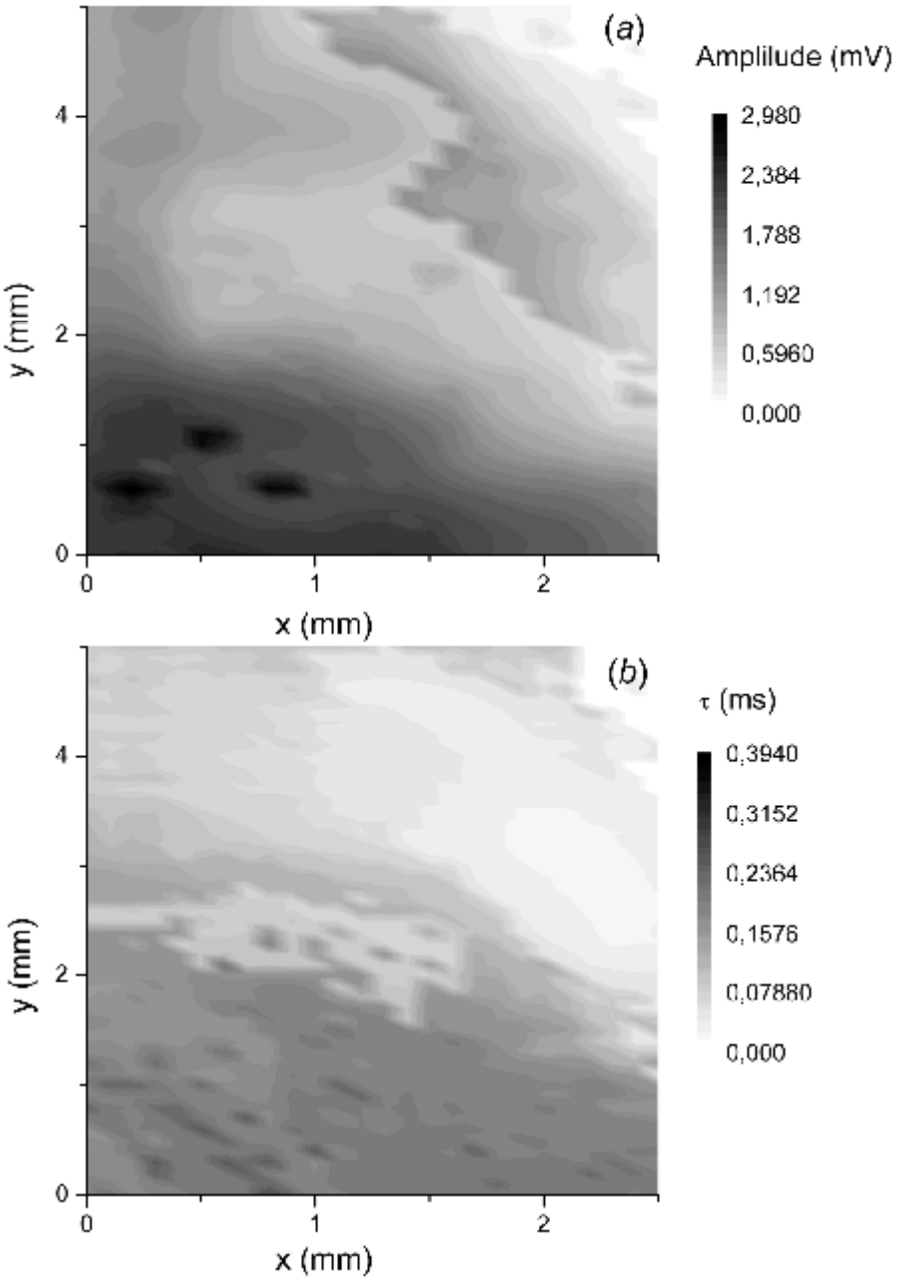

Fig. 4. Spatially resolved SPV amplitude U_0 (*a*) and decay time *t* (*b*) observed in Si-SiO_2-Ge sample

Ge heterostructure by taking surface distributions of the SPV signal. It is well known that the PV signal produced by the photoinjected carriers is basically due to contributions of the total amount of charge, and the distance between the centers of charge of the positive and negative carriers [8]. Therefore, the complexity of the confinement situation for electrons and holes in the Si-SiO_2-Ge structure shown in Fig. 2 indicates that the strain relaxation given above would be monitored within the framework of separated photoinduced charges and their time evolution detectable by measuring the SPV size and its transient.

The SPV amplitude U_0 and decay time t, taken in the substrate and in the Si-SiO_2-Ge sample, are mapped and the results are shown in Figs. 3 and 4, respectively. It is seen that both t and U_0 are much more non-uniform in the Si-SiO_2-Ge structure [images (*a*) and (*b*) in Fig. 4] than in the substrate [images (*a*) and (*b*) in Fig. 3], implying the existence of distributed sites affecting carrier lifetimes and SPV signals in Si-SiO_2-Ge. This is obviously consistent with the general view of the above calculations, illustrating an increase in the charge separation lengths due to QDs yielding non-uniform PV sizes and decay times. This observation can then be given a quantitative estimate in terms of the lengths of distributed sites capturing the carriers and the population of charges captured by the sites.

Conclusions

The influence of a thin SiO_2 layer, placed between the Si substrate and Ge quantum dot, on the strain relaxation inside the substrate is computationally investigated employing FEM techniques. Concomitant modifications of the band structure near the interface are also analyzed. Experimental surface distributions of the surface photovoltage signal give a general framework of a spatial distribution of the photogenerated electrons and holes near the interface relevant to the generation of capturing potential caused by the dots.

Курилюк В.В. - кандидат фізико-математичних наук, асистент кафедри фізики металів
Коротченков О.О. - доктор фізико-математичних наук, професор, професор кафедри загальної фізики;
Надточій А.Б. - кандидат фізико-математичних наук, молодший науковий співробітник кафедри загальної фізики. .

[1] F. Boxberg, J. Tulkki. Reports on Progress in Physics. 70(8), 1425 (2007).
[2] J.D. Cressler and G. Niu. Silicon-Germanium Heterojunction Bipolar Transistors. (Artech House, Norwood, 2003).
[3] V. Kuryliuk, O. Korotchenkov, A. Cantarero. Physical Review B. 85(7), 075406-1 (2012).
[4] C. Munakata, S. Nishimatsu, N. Honma, K. Yagi. Japanese Journal of Applied Physics. 23(11), 1451 (1984).
[5] A. Podolian, V. Kozachenko, A. Nadtochiy, N. Borovoy, O. Korotchenkov. Journal of Applied Physics. 107(9), 093706-1 (2010).
[6] P. Edelman, J. Lagowski, L. Jastrzebski. Materials Research Society Symposium Proceedings. 261(1), 223 (1992).
[7] C. Munakata, K. Yagi, T. Warabisako, M. Nanba, S. Matsubara. Japanese Journal of Applied Physics. 21(4), 624 (1982).
[8] I. Mora-Sero, Th. Dittrich, G. Garcia-Belmonte, J. Bisquert. Journal of Applied Physics. 100(10), 103705-1 (2006).

В.В. Курилюк, О.О. Коротченков, А.Б. Надточій

Релаксація деформацій у гетероструктурах Si/Ge з квантовими точками

Київський національний університет імені Тараса Шевченка,
вул. Володимирська, 64, Київ, 01601*; e-mail: kuryluk@univ.kiev.ua*

З використанням методу скінченних елементів чисельно досліджено вплив тонкого шару SiO_2, розташованого між підкладкою Si і Ge квантовими точками на релаксації напружень в підкладці. Також аналізуються супутні зміни зонної структури поблизу границі розділу. Експериментальні розподіли поверхневої фото-е.р.с. по поверхні зразків дозволяють виявити загальну структуру просторового розподілу фотогенерованих електронів і дірок поблизу границі розділу, що має відношення до розподілу центрів захоплення.

Ключові слова: квантова точка, напруження, релаксація, фото-ЕРС.