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THE SPATIAL SEPARATION OF ELECTRON-HOLE PAIRS IN Si/Ge HETEROSTRUCTURES

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Photogeneration and transport of nonequilibrium charge carriers, and the determination of photoresponce mechanisms in semiconductor SiGe/Si and SiGe/SiO_2/p-Si heterostructures with nanoisland were investigated. The structures were grown by molecular beam epitaxy technique. The work generalizes the results of studies of morphological, structural, optical and electrical properties of heterostructures with nanoscale objects – quantum dots and quantum wells. It is shown that the photoconductivity of nanoheterostructures SiGe/Si in the infrared range depending on the component composition, size and magnitude of the mechanical stresses in nanoislands $Si_{1-x}Ge_x$ is determined by interband and intraband transitions involving localized states of the valence band of the Ge nanoscale objects. The effects of long-decay photoconductivity and optical quenching of conductivity in SiGe/SiO_2/p-Si heterostructures with SiGe nanoclusters was found to be caused by variations of the electrostatic potential in the near-suraface region of p-Si substrate and optically-induced spatial redistribution of trapped positive charges between SiO_2/Si interface levels and localized states of Ge nanoislads.

*Adsorption complexes of germanium on the reconstructed Si(001)(4×2) surface have been simulated by the $Si_{96}Ge_2H_{84}$ cluster. For Ge atoms located on the surface layer of the latter, DFT calculations (B3LYP, 6-31G**) of their 3d semicore-level energies have shown a clear-cut correlation between the chemical shifts and mutual arrangement of Ge atoms.*

Introduction

Germanium nanoclusters grown on/in silicon have been successfully applied in new optoelectronic, and memory devices. Due to spatial confinement of charge carrier’s motion in one, two or three directions, respectively, such nanostructures have unique fundamental properties and technological applications [1, 2]. Of particular interest is attracted by nanoelectronic devices and systems grown using epitaxy methods - vapor-phase, molecular-beam and liquid-phase - in which the formation and spatial arrangement of nanoscale elements was carried out using the effects of self-organization.

In heterosystem Si/Ge with nanoislands distributed across the surface of inherent nonuniform field of mechanical stresses. Interfaces and their quantum-size classes, wetting layer (WL) heterogeneity leads to spatial heterogeneity of local electro-physical properties of Ge nanoclusters and induced spatial variation of the electrostatic potential. These features, expectedly, will have an impact on the transport of charge carriers along the epitaxial layers.

Heterojunctions Si / Ge are reffered to the second type , in which there is a limitation of motion of holes in Ge nanoclusters. That's why Ge nanoclusters can be considered as a long-term trap for holes, charge which a due to downward band bending in the underlying Si.

Semiconductor heterostructures and especially semiconductor heterostructures with low-dimensional objects, including quantum wells, quantum wires and quantum dots, currently comprise the object of intensive study [1, 3]. Of particular interest is attracted by nanoelectronic devices and systems grown using epitaxy methods - vapor-phase, molecular-

beam and liquid-phase - in which the formation and spatial arrangement of nanoscale elements was carried out using the effects of self-organization. Knowledge of the electronic spectrum, transport, recombination, and photogeneration in self-organized nanostructures is essential for creation of novel electronic and photonic devices.

Low-dimensional Ge/Si heterostructures have attracted considerable research interest in recent years, due to their significant potential to impact new electronic devices which are compatible with the available silicon technology. Optoelectronic devices based on SiGe dots grown on a Si substrate have been already proposed [4, 5]. The low-dimensional silicon-germanium alloys have a wide range of applications, including quantum dot IR photodetectors, memory cells and spintronic devices. Widespread application of such system is the arrangement of SiGe quantum dots in the space-charge region of heterojunctions, Schottky diodes, p-n junctions or metal-oxide-semiconductor structures.

Experiment

The molecular beam epitaxy (MBE) technique ("Katun'-B" set-up, produced in Novosibirsk, Russia) was used to prepare multilayer Ge-Si(100) nanocluster arrays with the islands of various sizes and surface density. The (100) oriented wafers of n-Si with 7.5 and 20 Ohm·cm resistivity and diameter of 76 mm were used as substrates. In order to prepare multilayer quantum dot systems with regular nanoisland distribution over the substrate surface, we have proposed to use a system of $Si_{1-x}Ge_x$ intermediate layers with a sub-critical thickness [5]. The Ge mole fraction x was gradually increased from layer to layer grown at gradually decreasing substrate temperature started from T_s=500 ºC. The growth process, in particular the moment of the $2D \rightarrow 3D$ transition in the Stranski-Krastanov growth regime, was controlled *via* RHEED (reflection high energy electron diffraction). To study the surface morphology, atomic force microscopy (AFM) measurements were carried out using an Ntegra AFM from NT-MDT with a closed loop scanner. Standard Si cantilevers with tips having a half opening angle of 10° were employed as probes. The growth of each Si intermediate layer was continued until a high-contrast Si(100)2×1 RHEED pattern was produced typical of clean Si. Thus, the multilayer Ge-Si(100) nanocluster arrays were grown at the temperature T_s=500 ºC.

The Stranski-Krastanow growth of Ge nanoislands on Si(001) surface is an intermediary process characterized by both 2D WL and 3D island formation. Transition from the layer-by-layer epitaxy to nanoisland structure growth occurs at a critical layer thickness which is highly dependent on surface energies and lattice parameters. Germanium nanoclusters grown on/in silicon or silicon dioxide have been successfully applied in new nanoelectronic, optoelectronic and memory devices due to quantum confinement effect and possibility of integration within Si-based technology.

Micro Raman scattering spectra of the investigated structures were recorded at room temperature using automated Raman diffraction spectrometer T-64000 Horiba Jobin-Yvon equipped with CCD detector. The line 488 nm of Ar-Kr laser of 3 mW was used for excitation. Raman spectra were measured for the geometry $z(x,y)$ - x, where axes x, y, z correspond to [100], [010] and [001] crystallographic directions, correspondingly. Ohmic Au–Si contacts of rectangular shape and dimensions of 4x1 mm were welded into epitaxial layers at 370 ^{0}C for lateral photoconductivity measurements. The distance between contacts on the sample surface was 5 mm. Current-voltage characteristics of the structures studied were found to be linear in the range from –10 V to +10 V at temperatures between 50 and 290 K. Lateral photoconductivity spectra were measured at excitation energies ranging from 0.48 to 1.7 eV under illumination with a 250-W halogen lamp. The corresponding direct photocurrent signal was registered by a standard amplification technique. Spectral dependences were normalized to the constant number of exciting quanta using anonselective pyroelectric detector.

Non-epitaxial Ge nanoislands which are separated from the substrate attract special interest due to spatial separation of electron-hole pairs leading to reduction of recombination rate. NI's growth at the silicon surface covered with ultrathin silicon oxide layer is mainly determined by the dynamics of changes of the SiO_x film structure and physical properties during Ge deposition and is principally possible at temperatures below ~400 ºC, when the formation of voids in ultrathin SiO_2 films is suppressed. Epitaxy at such low temperatures puts some limitations on the crystallinity and structural perfection of the obtained nanoclusters. Increasing of growth temperature up 430 ºC allows to grow epitaxial crystalline NI's on silicon, while silicon oxide is destroyed due to thermal decomposition effect.

Results and discussion

Fig. 1a shows AFM image of the top layer of a typical sample with one layer of nanoislands large scatter and significant in size. The figure shows that the surface contains nanoislands size of the basics about 98 nm and a height of about 15 nm. The average surface density of nanoislands is ~ 10^{10} cm^{-2}. Composition and values of elastic strains in investigated Ge/Si heterostructures were estimated using Raman spectroscopy. Typical Raman spectrum of Ge/Si heterostructure containing 5 layers of Ge quantum dots is given in fig. 1b. It contains phonon bands corresponding to Ge-Ge, Si-Ge and Si-Si vibrations, which is typical for SiGe heterostructures with nanoislands, which makes possible to estimate content and strain values for Ge nanoislands [9]. Thus, Ge mole fraction and elastic strains in Ge nanoislands were found to be $x = 0.91 \pm 0.02$ and, $\varepsilon_{xx} = -0.01$, correspondingly.

The $Si_{1-x}Ge_x$/Si heterostructures are refered to the second type, in which the potential well for holes is in the valence band of $Si_{1-x}Ge_x$ (Fig. 2a). Energy diagram of the heterojunction is primarily determined by the values of the band gap and electron affinity of the contacting materials. In unstrained $Si_{1-x}Ge_x$ alloys the bandgap decreases monotonically with increasing of Ge content. Fig. 2b shows the results of numerical calculations of the energy spectra of holes in $Si_{1-x}Ge_x$ quantum wells with width of 2 nm for different Ge contents. The analysis shows that the energy position of localized states with respect to top of Si valence band increases nonlinearly with x due to the dependence of the effective mass of holes from the strain values in this system. Deep potential well in the valence band favor to accumulation of holes in Ge nanoislands in the wide temperature range. In the other word, the Ge nanoislands can be considered as a giant traps for holes. Positive charge of trapped holes induces downward band bending in the underlying *p*-Si substrate. Moreover, the band bending expected to be larger in the region beneath of nanoisland base.

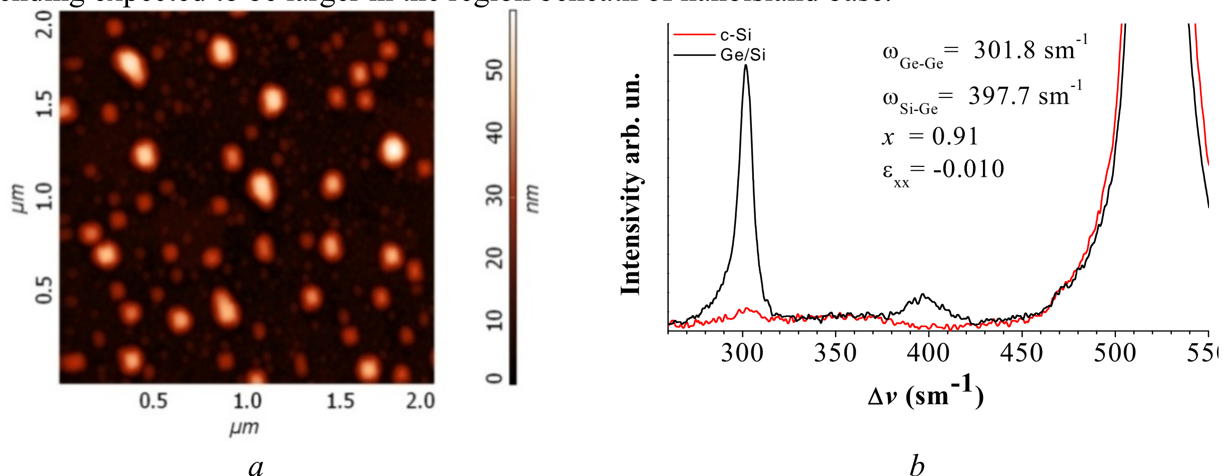

Fig. 1. The AFM image of the surface of nanoislands Ge, grown by MBE at 500 º C on the surface of the substrate p-Si (001) (a) and Raman spectra (b) Si / Ge heterostructure with nanoislands $Si_{1-x}Ge_x$ on the substrate p-Si (001) (sample 302.03.11).

Analyzing the energy diagrams of $Si_{1-x}Ge_x$/Si heterojunction we can conclude that the photosensitivity range of these structures is determined by the position of the Fermi level in the heterostructure, i.e. the concentration dopant in Si substrates and epitaxial films. Interband optical transitions are realized in the presence of electrons in quantum-sized states of the valence band nanoislands. For intraband transitions in the valence band, the Fermi level must be below at least the ground state of nanoislands. Development of efficient optoelectronic devices requires information on energy, oscillator strengths, and selection rules for interband and intrabend transitions. Fluorescent measurements do not reflect all transitions possible in heterogeneous in size and composition of deformations heterostructures. Opportunities of absorption spectroscopy are severely limited by the fact that the passage of radiation through nanoscale quantum dot layer is absorbed only by its small part (~ 10^{-4} - 10^{-5}). As a result, the direct measurement of the absorption spectra of quantum dots is rather difficult task which requires a very sensitive technique and long-time measurements. One of methods which makes possible to study the absorption spectra in nanoscale semiconductor structures is an in-plane photocurrent spectroscopy. The value of photoconductivity is proportional to the number of photogenerated charge carriers, and thus the absorption coefficient. Photocurrent spectroscopy is a direct, sensitive and relatively simple method of studying the shape of optical absorption spectra and energy and interband transitions possible in heterostructures with nanoscale objects.

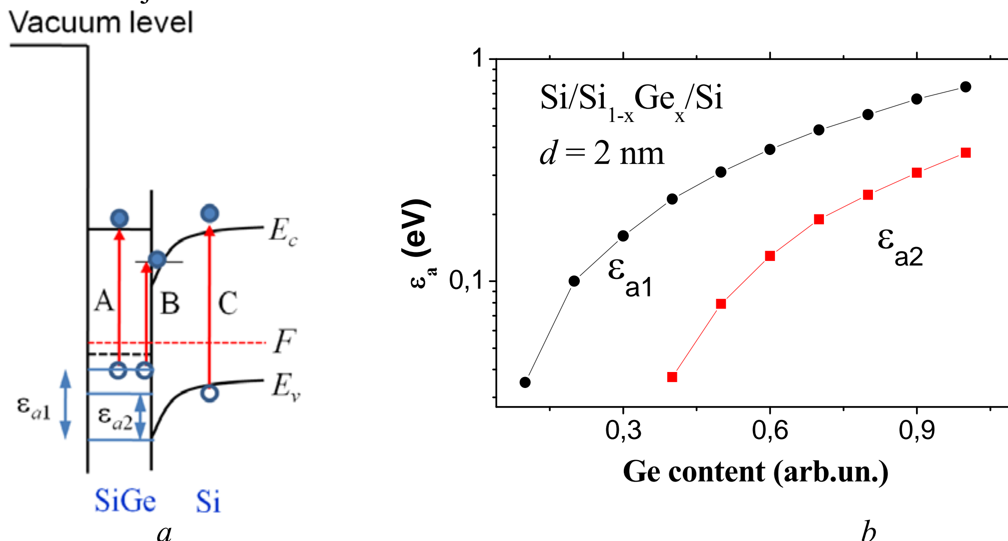

Fig. 2. Energy diagram of Si/Ge heterostructures with Ge nanoislands (a). The activation energies for localized holes of $Si_{1-x}Ge_x$ quantum wells with width of 2 nm and different content of Ge (b).

Excitation of nonequilibrium charge carriers in Si/Ge heterostructures with Ge nanoislands causes conductivity changes in the space charge region of *p*-Si transport channel. Photoconductivity spectra (Fig. 3a) measured at excitation and steady temperatures 50-80-120 K contained two components. At $h\nu > \varepsilon_{g,\ Si}$ (1.16 eV at 50 K), the main contribution to the photoconductivity gives electron-hole pairs photoexcited in the substrate *p*-Si due to interband transitions (see transition C in Fig. 2a).

In the spectral region where Si is transparent, photoconductivity originates from interband electronic transitions involving localized states nanoislands $Si_{1-x}Ge_x$. The monopolar photoconductivity was observed in this case. Interband electronic transitions between localized states of the valence band of SiGe nanoislands and delocalized states of the conduction band of silicon surrounding can be observed in low-dimentional Si-Ge heterostructures. The spectral range of interband transitions is determined by Ge contents of QDs, strain values, and confinement energy for holes in the valence band [10]. Transitions A

and B (Fig.2a) are possible if ground states are partially filled by electrons. These transitions cause the appearance of nonequilibrium electrons in the Si spacer layers and WLs, which are transport channel, while photoexcited holes are localized in Ge.

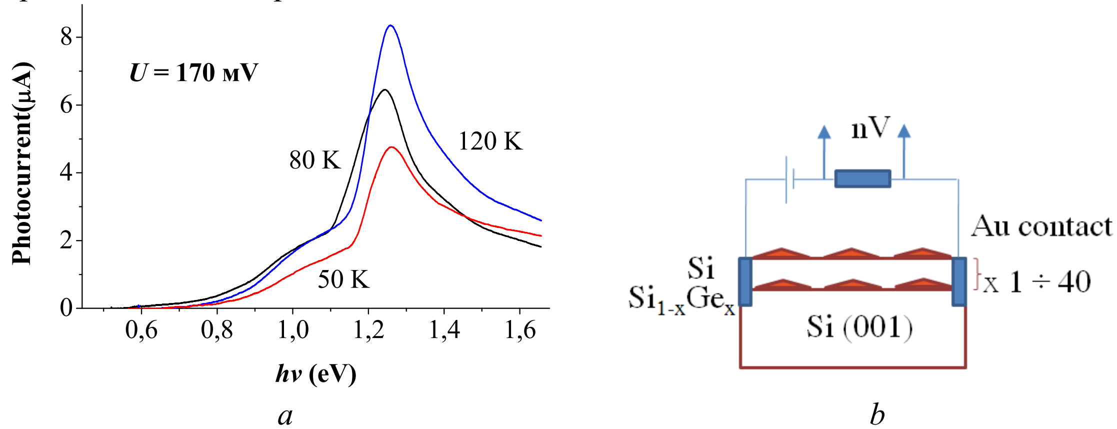

Fig. 3. Photoconductivity spectra of Si / Ge heterostructure with nanoislands $Si_{1-x}Ge_x$ on the substrate p-Si (001).

Measurements of infrared photoconductivity in Ge-NC/SiO_2/Si structures made it possible to evaluate their electronic spectrum. The PC spectra measured at temperatures 50, 80, and 120 K (Fig.4) give information about energies of electronic transitions in Ge-NC/SiO_2/*p*-Si structure. The in-plane photocurrent in the range $h\nu > \varepsilon_{G,Si}$ is mainly originated from band-to-band transitions in *c*-Si. For light excitations with photon energy below band gap of Si $h\nu < \varepsilon_{G,Si}$ ($\varepsilon_{G,Si}$=1.17 eV at 77 K), the electronic transitions from valence band to conduction band of NCs give main contribution to PC. However, generation of photocurrent in the range $0.8 < h\nu < \varepsilon_{G,Si}$ for Ge-NC/SiO_2/Si is also possible due to transitions between tails of the density of states in the near-surface *c*-Si [11], the optical absorption spectra of which are described by Urbach law. The electron transitions through the states of Ge-NC/SiO_2 and Si/SiO_2 interfaces may also be observed, however their contribution to PC is expected to be small due to high probability for recombination through interface state.

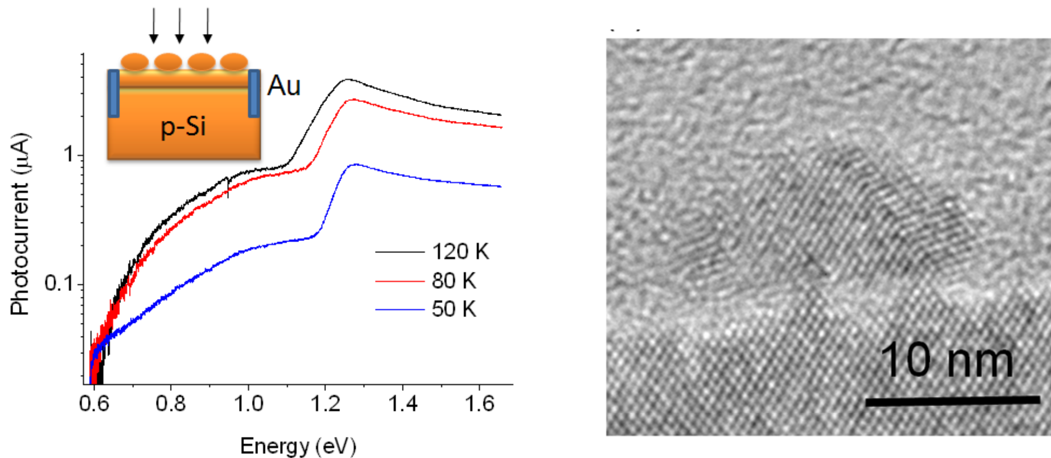

Fig. 4. In-plane PC spectra of Ge-NC/SiO_2/Si measured at 50 K, 80 K, and 120 K and HR-TEM images of Ge NCs grown on silicon oxide.

The contribution of electron-hole pairs photoexcited in Si is observed, when the quanta energy exceed the band gap value. In the spectral range $h\nu < 1.1$ eV, in which *c*-Si is transparent, interband indirect transitions take place via the states in the valence and conduction bands of nanoclusters. Non-equilibrium carriers photoexcited in nanoclusters do not contribute into carrier transport directly. In order to contribute into the lateral current, the non-equilibrium electrons and holes should be spatially separated. As for Ge/Si

heterojunctions, studied systems referred to type II, where strong confinement for holes in the region of Ge nanoclusters occurs. In the studied heterostructures, electrons can tunnel through the oxide SiO_x film into the near-surface silicon region and make contribution into conductivity. At the same time, non-equilibrium holes are localized in the valence band of Ge nanoclusters, however, they can affect the potential relief in the near-surface region of Si substrate, and hence, make an indirect effect on the system conductivity.

Thus, photoconductivity of the structures in the range of Si transparency is unipolar – intrinsic absorption of light in nanoclusters leads to an increase of the electron concentration in the Si potential well near the SiO_x-Si interface and to an increase of the surface conductance. In this case, the shape of lateral photoconductivity spectra reflects main features of intrinsic absorption of light in nanoclusters. The edge of PC spectrum of the investigated structures at $h\nu > \varepsilon_0$ is described by the dependence typical for the indirect band semiconductors:

$$\alpha(h\nu) = \frac{C}{h\nu}(h\nu - \varepsilon_0)^2 , \qquad (1)$$

where C is a constant, ε_0 is the width of the optical band gap. At excitement with quanta $h\nu<\varepsilon_0$ the Urbach tail is observed due to the crystal structure disorder.
Photocurrent spectroscopy and X-ray diffraction demonstrate that the nanoclusters have the local structure of body-centred-tetragonal Ge, which exhibit an optical adsorption edge at ε_0 = 0.48 eV. Taking into account quantum-size effect, this is in a good agreement with the theoretical calculations of electronic and optical properties of bulk body-centered-tetragonal Ge and Si, according to which the band gap width for the mentioned polytypes is 0.38 and 0.86 eV, respectively [12].

Influence of the localization of Ge atoms within the Si(001)(4×2) surface layer on semicore one-electron states. A number of parallel or sequential processes normally occur as soon as a heterojunction between a germanium quantum dot and reconstructed Si(001)(4×2) surface is formed [13, 14]. The most important of those processes is the formation of >Ge–Ge< surface dimers on the top of a series of asymmetric >Si–Si< species located on the buckled surface. Taking into account a similarity between Si and Ge covalent radii (1.17 and 1.22 Å, respectively [16]), a diffusion penetration of Ge atoms into the crystalline substrate simultaneously with a displacement of an equivalent amount of Si atoms towards the surface may take place. As the result, a formation of mixed >Si–Ge< surface dimers is possible. Together with the thermal motion, those processes reduce the abruptness of the Ge/Si heterojunction [17, 18] and hence deteriorate the robustness of corresponding solid state electronic devices. Therefore, a reliable location of the Ge sites on the Ge/Si interface between a germanium quantum dot and Si(001)(4×2) crystalline substrate presents an important task.

For such molecular systems as solid-state adsorption complexes, the most precise and exhausting information on the local environment of atoms can be extracted from photoelectron spectra [13]. In particular, the latter can be adequately interpreted in terms of the density of one-electron states over a wide energy range, as soon as corresponding theoretical models are available [19, 20]. The interpretation of photoelectron spectra is facilitated by their classification into three regions according to the binding energies of electrons (E_i) [19]. The first region (0 ÷ 5 eV) includes a poorly resolvable and rather complicated structure due to the electrons from valence molecular orbitals (MOs) that mainly consist of the atomic orbitals (AOs) belonging to partially occupied electron subshells. The structure of the second region (ca. 15 ÷ 50 eV) is usually well resolved and can be associated

with the linear combinations of semicore AOs originating from closed (sub)shells. The latter, in contrast to valence AOs, in some cases can be combined to so-called internal MOs (IMOs) [21, 22]. In the case of adsorption complexes, the formation of those IMOs can be monitored by the exaggerated binding energies of adatoms. Finally, the lines belonging to the third region of photoelectron spectra (> 50 eV) are almost solely associated with the core-shell (deep-core) AOs that normally do not contribute to IMOs.

In this paper we report on the calculated densities of one-electron states for a number of clusters with the same brutto formula $Si_{96}Ge_{2}H_{84}$. Thus, so-called cluster A (Fig. 5) simulates a fragment of the Si(001)(4×2) relaxed surface with the >Ge–Ge< surface dimer located over the series of >Si–Si< surface dimers. Clusters A1, A2, A3, and A4 correspond to different localizations of Ge atoms within the subsurface region of the substrate.

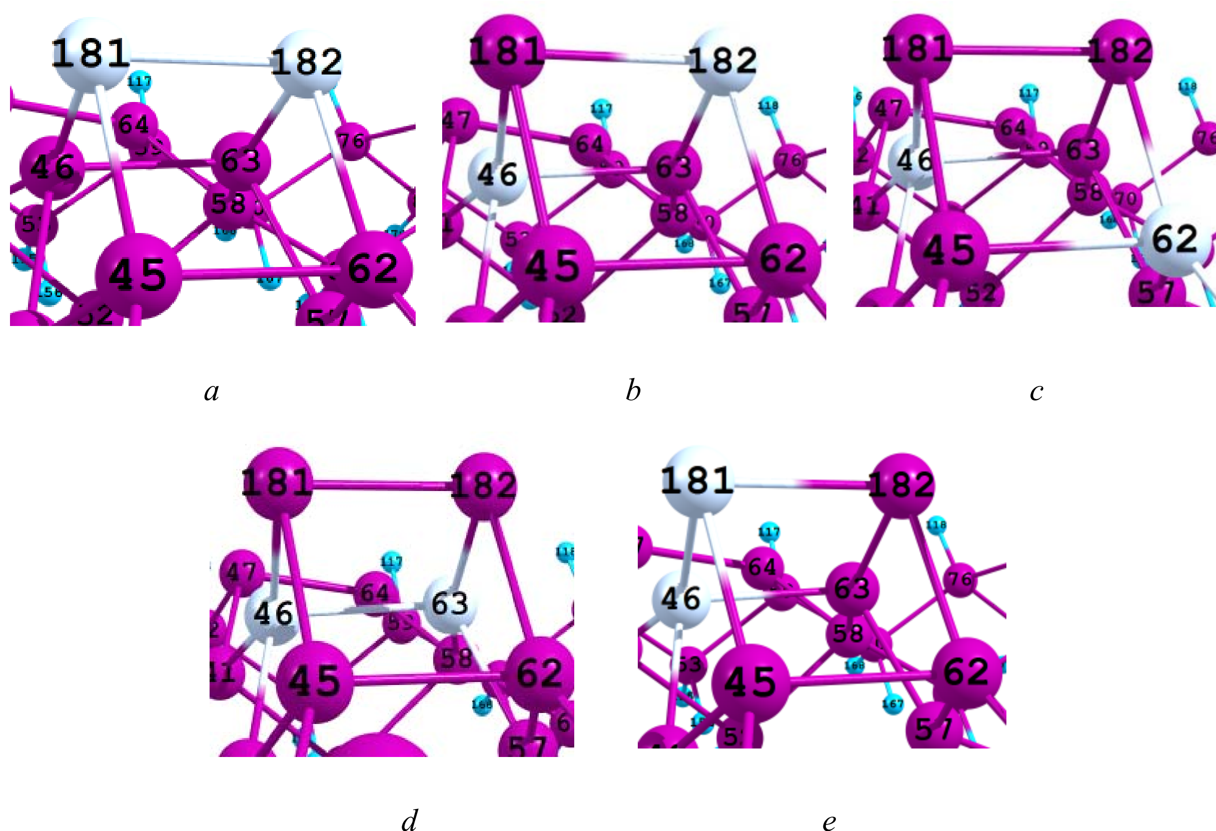

Fig. 5. *a* – Configuration of the adsorption complex A ($Si_{96}H_{84}\bullet Ge_{2}$) with a pure >Ge–Ge< dimer on the top of a series of surface >Si–Si< dimers; *b* – Cluster A1; *c* – Cluster A2; *d*– Cluster A3; *e* – Cluster A4. Clusters A1÷A4 are formed from Cluster A as the result of a substitution of one or two surface Ge atoms by Si atoms of the substrate.

Calculations of the equilibrium geometry and electronic structure of these clusters have been performed within the framework of Kohn-Sham density functional theory, using hybrid B3LYP exchange-correlation functional [23-26] and 6-31 G** basis set. General Atomic and Molecular Electronic Structure System (GAMESS) suite of programs [27] has been employed.

We have shown in our previous study [28] that cluster A characterized by a pure >Ge–Ge< surface dimer is the most stable, while total energies of clusters A1 ÷ A4 with either pure >Si–Si< surface dimer (A2 and A3) or mixed >Si–Ge< one (A1 and A4) are somewhat higher. Therefore, the substitution of germanium atoms in a >Ge–Ge< dimer by one or two substrate silicon atoms is an endothermic process (see Fig. 5 and Table 1).

The density of one-electron states of the $Si_{96}H_{84}Ge_2$ cluster (Fig. 6) shows a bimodal shape for 2*s* and 3*s* lines originating from the non-equivalency of Ge atoms within the >Ge-Ge< surface dimer of the reconstructed Si(001)(4×2) surface, one of those Ge atoms being in a so-called *down*-, and another in *up*-position [28].

Table 1. Calculated relative energies of Clusters A1÷A4 and chemical shifts for the $3d_{5/2}$ component of the Ge($3d$) line. Cluster A is taken as the reference (see Fig. 5).

Cluster	A1	A2	A3	A4
Relative energy, kcal/mol	1.83	5.15	2.72	5.11
Chemical shift, eV	+0.12	-0.08	-0.07	+0.10

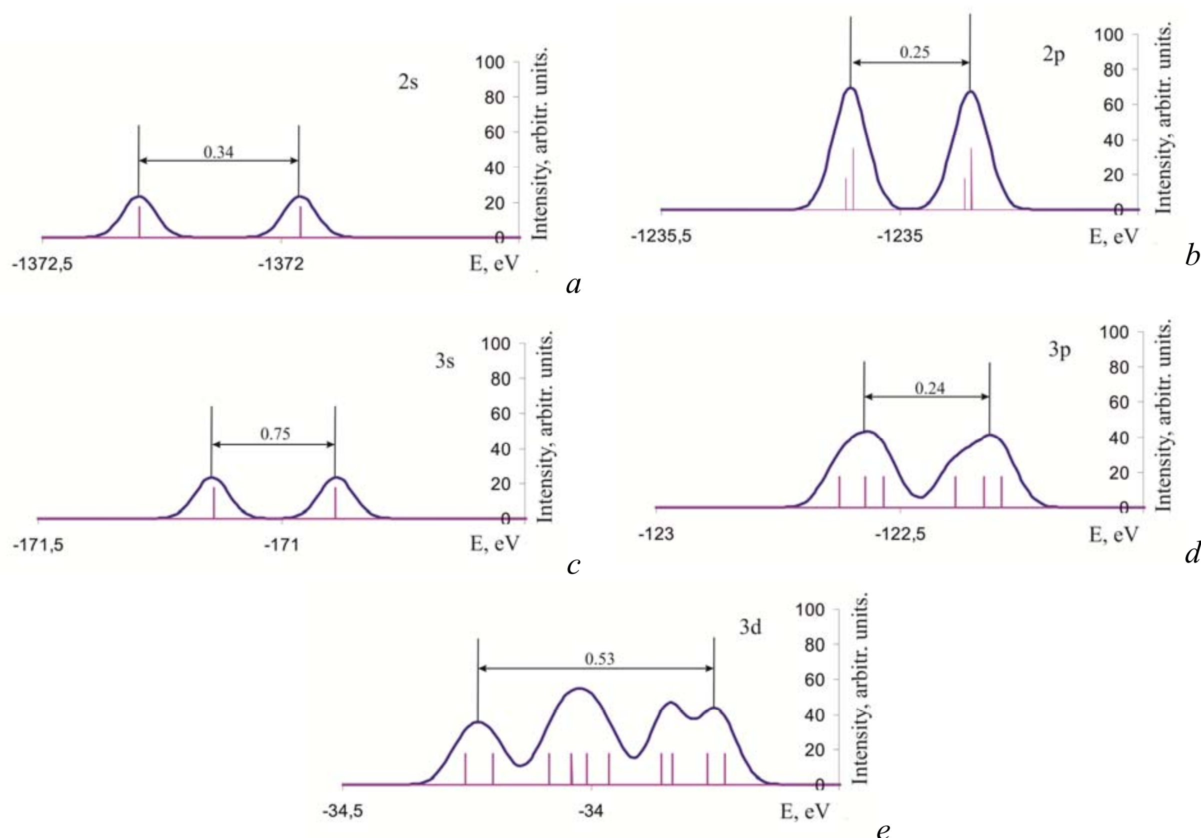

Fig. 6. Density of the core one-electron states for Cluster A within the binding-energy ranges of (*a*) 2s, (*b*) 2p, (*c*) 3s, (*d*) 3p, and (*e*) 3d electrons of the Ge atom.

Moreover, the intensities of $2p_{3/2}$ and $2p_{1/2}$ components are essentially the same, as well as those of $3p_{3/2}$ and $3p_{1/2}$, that contradicts theoretical expectations based on the population of the corresponding levels (in contrast to the isolated Ge_2 molecule where those expectations are justified). The Ge(3*d*) line deviates from the bimodal shape and, to a certain extent, keeps the shape motif of the corresponding line of Ge_2 molecule. It is important to note that not only the IMO formation but also the abovementioned non-equivalence of Ge atoms within the >Ge–Ge< surface dimer sophisticates the shape of the Ge(3*d*) line. That might indirectly confirm the presence of Ge_2 molecules within the adsorption phase of the Si(001)(4×2) surface, despite the calculated Ge–Ge bond lengths are 2.16 Å and 2.21 Å in the >Ge–Ge< surface dimer and in the isolated Ge_2 molecule, respectively.

Analysis of the deep-core and semicore-electron densities of states within the energy ranges of germanium 1*s*, 2*s*, 2*p*, 3*s*, 3*p*, and 3*d* levels indicates the position of 3*d* level to be

the most sensitive one with respect to the mutual arrangement of Ge and Si atoms within all the clusters under consideration.

Calculated energy shifts of the spin-orbit component $3d_{5/2}$ in Clusters A1÷A4 relative its position in Cluster A (Table 1) shows that the migration of germanium atoms from the >Ge-Ge< surface cluster into the bulk substrate increases the absolute values of 3*d* binding energies for Clusters A1 and A4 (one Ge atom is within the mixed >Si–Ge< surface dimer, and another is in the bulk), but decreases them for Clusters A2 and A3 (pure >Si–Si< surface dimer and both germanium atoms are in the bulk). Such an effect is less pronounced in the latter case.

According to the scheme accepted, a binding energy of a semicore electron is determined by two factors: (i) formal oxidation state of an atom which can be identified with its formal charge, and (ii) relative donor-acceptor properties of this atom as well as those of its neighbors.

Two germanium atoms (Nos. 181 and 182) (fig. 5) entering the >Ge–Ge< dimer in Cluster A are charged negatively, while the sum of charges on their neighbors is positive. In Cluster A1, Ge(46) atom is embedded into the substrate, and its negative charge increases to -0.081 atomic units (a. u.) (that of Ge(182)) amounts to -0.065 a. u.), while the positive sum of charges on the neighboring atoms (0.074 and 0.118 a. u. for Ge(46) and Ge(182), respectively) increases as well comparing to Cluster A. As the result, a positive chemical shift of the semicore-electron binding energy relative Cluster A is observed.

Cluster A2 contains Ge(46) and Ge(62) atoms within the crystalline substrate, whose charges are -0.023 and -0.010 a. u., respectively, while the sum of charges on neighboring atoms is also positive, but significantly smaller than that for Cluster A. According to the electrostatic potential approximation, that leads to a negative chemical shift, as one could expect.

The situation seems to be more complicated for Cluster A3 because of an invariance of the charge on Ge(46) comparing to Cluster A, and a decrease of the negative charge on Ge(63) to -0.006 a.u. Together with a negative sum of charges on neighboring atoms, these circumstances enhance the role donor-acceptor properties of surrounding silicon atoms and thus explain the negative chemical shift.

In Cluster A4 Ge atoms are directly bonded to each other, while one of them Ge(181) enters >Si–Ge< mixed dimer and another Ge(46) is located within the crystalline substrate. The charge of the latter atom amounts to -0.118 a. u., and the sum of charges on its neighbors is +0.116 a. u. Such a charge distribution (similar to that of Cluster A1) results in a positive $3d_{5/2}$ chemical shift of the $\mathrm{Ge}(3d)$ line.

Conclusions

The mechanism of photoconductivity in the Ge/Si generally, which are referred to the second type heterostructures, depends on quantum energy of exciting illumination. The lateral photoconductivity observed in the range 0.63 – 1.0 eV below fundamental absorption edge of c-Si was caused by interband transitions from the ground state of a Ge nanoislands to the conduction band of a silicon surrounding. Photoexcited holes was found to be localized in Ge nanoislands, while photoelectrons are supposed to be free in the conduction band of Si giving contribution to the monopolar photoconductivity. In the case of excitation of Ge/SiO_2/Si structures an interband transitions in Ge create localized holes in Ge directly, leading to optically-induced spatial redistribution of trapped positive charges between SiO_2/Si interface levels and localized states of Ge-NCs, which enhance variation of electrostatic potential in underlying Si and, therefore, decay of surface conductivity under stationary photoexcitation. Observed results demonstrate that hole trapping by Ge-NCs and interface states have a significant effect on in-plane transport in the Ge-NCs/SiO_2/Si structures.

The comparison semicore-level energy shifts for adsorption complexes simulated by a series of clusters with the same brutto formula $Si_{96}Ge_2H_{84}$ but different arrangements of germanium atoms within the surface layer and bulk with a similar spectrum of the Ge_2 molecule has led us to the following conclusions:

(i) Atomic orbitals from the closed d shell of germanium atom contribute to internal molecular orbitals that are responsible for a high binding energy of the >Ge–Ge< surface dimer.

(ii) For $Si_{96}Ge_2H_{84}$ clusters containing one germanium atom embedded in a crystalline silicon substrate, a $3d_{5/2}$ chemical shift of the Ge($3d$) line is positive (i. e., the binding energy of the corresponding electrons is higher comparing to that in the cluster containing >Ge–Ge< surface dimer). For clusters with both germanium atoms embedded in a substrate, such a chemical shift is negative.

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ПРОСТОРОВИЙ РОЗПОДІЛ ЕЛЕКТРОН-ДІРКОВИХ ПАР В Si/Ge ГЕТЕРОСТРУКТУРАХ

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Були досліджені фотогенерація і транспорт нерівноважних носіїв заряду і визначений механізмфотовідповіді в напівпровідникових SiGe/Si і SiGe/SiO$_2$/Sip-гетероструктурах з наноострівцями. Зразки були вирощені методом молекулярно-променевої епітаксії. У роботі узагальнені результати досліджень морфологічних, структурних, оптичних та електричних властивостей гетероструктур з нанорозмірними об'єктами – квантовими точками і квантовими ямами. Показано, що фотопровідність наногетероструктури SiGe/Si в інфрачервоному діапазоні в залежності від компонентного складу, розмірів і величини механічних напружень в

наноострівців $Si_{1-x}Ge_x$ визначається міжзонними і внутрізонними переходами за участю локалізованих станів валентної зони Ge нанорозмірних об'єктів. Були встановлені ефекти фото- довгострокового розпаду і оптичного затухання провідності в $SiGe/SiO_2/n$-Si гетероструктур з SiGe нанокластерами, які викликані змінами електростатичного потенціалу в приповерхневій зоні p-Si підкладки і оптично-індукованого просторового перерозподілу захоплених позитивних зарядів між рівнями межі розділу SiO_2/Si і локалізованих станів Ge наноострівців.

*Були вивчені адсорбційні комплекси германію на реконструйованій грані Si (001) (4×2) на прикладі кластера $Si_{96}Ge_2H_{84}$. Для атомів Ge, локалізованих в приповерхневому шарі кластера, результати розрахунків методом ТФГ (B3LYP, 6-31G**) положення їх 3d-остовних рівнів свідчить про кореляцію між хімічним зсувом Ge (3d) і хімічним оточенням атомів германію.*

ПРОСТРАНСТВЕННОЕ РАСПРЕДЕЛЕНИЕ ЭЛЕКТРОН-ДЫРОЧНЫХ ПАР В Si/Ge ГЕТЕРОСТРУКТУРАХ

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Были исследованы фотогенерация и транспорт неравновесных носителей заряда и определен механизм фотопроводимости в полупроводниковых SiGe/Si и $SiGe/SiO_2/Sip$-гетероструктурах с наноостровками. Структуры были выращены методом молекулярно-лучевой эпитаксии. В работе обобщены результаты исследований морфологических, структурных, оптических и электрических свойств гетероструктур с наноразмерными объектами – квантовыми точками и квантовыми ямами. Показано, что фотопроводимость наногетероструктуры SiGe/Si в инфракрасном диапазоне в зависимости от компонентного состава, размеров и величины механических напряжений в наноостровках $Si_{1-x}Ge_x$ определяется межзонными и внутризонными переходами с участием локализованных состояний валентной зоны Ge наноразмерных объектов. Были установлены эффекты фото долгосрочного распада и оптического затухания проводимости в $SiGe/SiO_2/n$-Si гетероструктур с SiGe нанокластерами, которые вызваны изменениями электростатического потенциала в приповерхностной зоне p-Si подложки и оптически индуцированного пространственного перераспределения захваченных положительных зарядов между уровнями границы раздела SiO_2/Si и локализованных состояний Ge наноостровков.

*Были изучены адсорбционные комплексы германия на реконструированной грани Si(001)(4×2) на примере кластера $Si_{96}Ge_2H_{84}$. Для атомов Ge, локализованных в приповерхностном слое кластера, результаты расчетов методом ТФП (B3LYP, 6-31G**) положения их 3d-остовных уровней свидетельствует о корреляции между химическим сдвигом Ge(3d) и химическим окружением атомов германия.*