A.A. GRYNCHUK, I.P. KOVAL, M.G. NAKHODKIN

Taras Shevchenko National University of Kyiv
(64, Volodymyrs'ka Str., Kyiv 01601, Ukraine; e-mail: greenchuckaa@gmail.com)

PACS 62.40.+i

SURFACE STRESSES AT THE INITIAL STEPS OF THE Ge_xSi_{1-x}/Si(001) SURFACE OXIDATION

Elastic stresses arising at the clean Ge_xSi_{1-x}/Si(001) surface, as well as at the initial stages of its oxidation, are considered qualitatively by analyzing the changes of unit cell dimensions occurring owing to the ad-dimer formation or the atomic or molecular adsorption on the unit cell surfaces. The stress character is found to be almost identical for the clean Ge_xSi_{1-x}/Si(001) surface and the Ge_xSi_{1-x}/Si(001) surface with adsorbed oxygen molecules or one to three adsorbed oxygen atoms. In addition, the surface stresses revealed a significant anisotropy: they turned out compressive along the dimer rows and three times as large as tensile stresses in the perpendicular direction (along the interdimer bonds).

Keywords: stress, stress anisotropy, oxidation.

1. Introduction

Large attention in modern nanoelectronics is paid to the heteroepitaxial growing of Ge on Si, since the hole mobility in the SiGe layer is higher than that in Si, the latter being mainly used in metal-oxide-semiconductor (MOS) devices [1]. In the manufacture of MOS facilities, an important role is also played by the oxide layer SiO_2. Therefore, the formation of an atomically controlled thin SiO_2 layer on silicon surfaces and the process of oxidation of stressed SiGe structures are important for the development and the functioning of modern nanoelectronic circuits.

In works [2–5], the oxidation process was considered for Si(001) surfaces with one or two monolayers of Ge atoms. It was shown that the coefficients of oxygen sticking to a clean Si(001) surface is by an order of magnitude higher than in the cases of Ge/Si(001) surface with one or two monolayers of Ge adatoms fabricated at 350 °C. If the same surfaces were fabricated at 600 °C, the sticking coefficient increased, but remained still lower than the coefficient of sticking to the clean Si(001) surface [3]. A reduction of the coverage degree of Si(001) surface by Ge atoms to a submonolayer ($\theta_{\mathrm{Ge}} < 1$) gave rise to the increase of the oxygen sticking coefficient to this surface [5]. In the opinion of the authors of work [5], this fact can result from the presence of additional surface stresses because of the lattice constant mismatch between Si and Ge. The influence of surface stresses and their anisotropy on the surface structure was established in work [6]. Surface stresses turned out to strongly affect the reconstruction of surface structures [7]. However, neither the character of those stresses nor their magnitude at complicated semiconductor surfaces after the oxygen adsorption has been determined till now. Therefore, to make the growth of thin oxide layers on the Ge_xSi_{1-x}/Si(001) surface more controllable, it is necessary to consider the character of stresses at the clean surface and at the initial stages of its oxidation. This task was the aim of this work.

2. Methods

2.1. Calculation routine

The surface stresses induced by the formation of ad-dimers on the Ge_xSi_{1-x}/Si(001) surface followed by the adsorption of O_2 molecules or individual O atoms on them were analyzed with the help of the ratios $\Delta a/c$ and $\Delta b/c$ between the deformations of lateral dimensions in a unit cell, Δa and Δb, and the corresponding quantities in the bulk Si(001), which are equal in this case and amount to c. The electron and geometry structures of the Ge_xSi_{1-x}/Si(001) surface were analyzed by carrying out *ab initio* calculations with periodic boundary conditions [8] in the density functional theory (DFT) approximation [9]. For the description of the exchange-correlation interaction, the generalized gradient approximation (GGA) [8] was used. The interaction between the core and valence electrons was described with the use of the

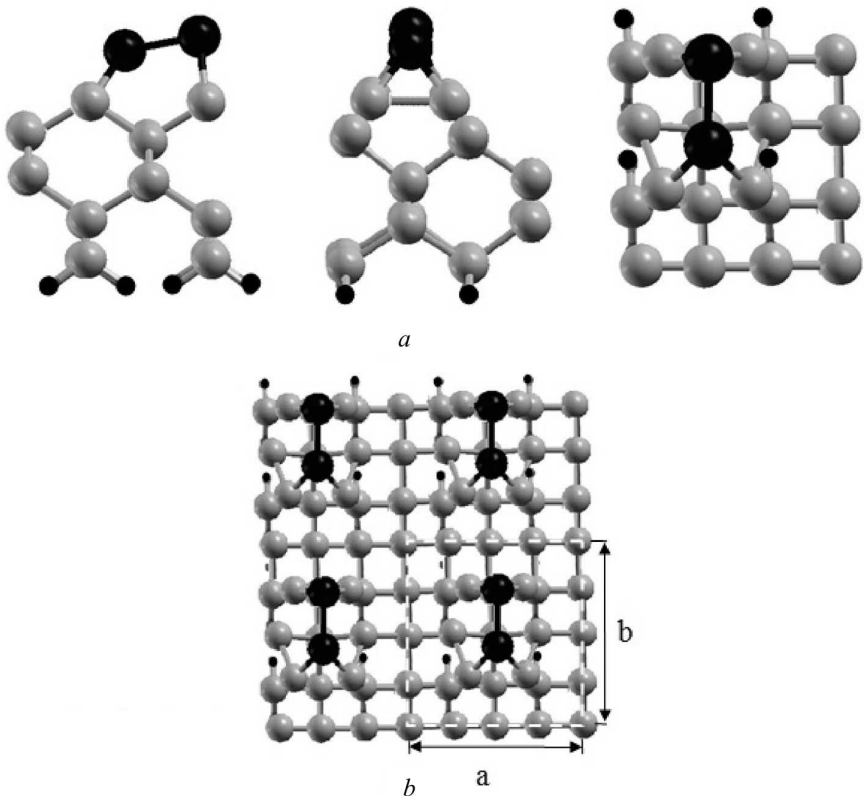

Fig. 1. Unit cell (views from both sides and a perspective one) chosen for simulating the $Ge_xSi_{1-x}/Si(001)$ surface (a) and its characteristic dimensions used while analyzing the surface stresses (b). Grey, large black, and small black beads denote Si, ad-dimer, and H atoms, respectively

norm-conserving pseudo-potential [8]. The calculations were carried out with the help of the software package *Abinit* [10].

The model of repeated plates was applied to simulate the surface. The plates had pure (Si–Si and Ge–Ge) or mixed (Si–Ge) ad-dimers (black beads in Fig. 1, a) adsorbed on the dimers of the Si(001) surface on one of the plate sides and H atoms, which saturated the dangling bonds on the other side. The number of atomic Si layers in the plate was determined by calculating the ratios $\Delta a/c$ and $\Delta b/c$. For unit cells with the number of atomic Si layers larger than 5, the corresponding values changed by no more than 10^{-3}. Therefore, to reduce the required calculation resource, we selected a unit cell that contained 5 atomic Si layers. Hence, a unit cell which could reproduce a layer contained 30 atoms (Fig. 1). To exclude the interaction between atoms belonging to different plates, the thickness of the vacuum gap between the latter was selected to equal 15 Å. The locations of atoms in five near-surface layers were iteratively optimized until the forces acting on the atoms became less than 0.03 eV/Å. The improvement of conditions for the convergence of the iterative procedure did not change the calculated values of energies for the systems under investigation and their geometrical parameters. The integration over the Brillouin zone was carried out with the help of a $2 \times 1 \times 1$-grid of special points and following the Monkhorst–Pack scheme [11]. In order to determine the cut-off energy, we calculated the binding energy between Ge atoms and the Si surface. For the cut-off energy equal or larger than 217.7 eV, this quantity was found not to change; therefore, all calculations were carried out for the indicated value.

The quantities $\Delta a/c = a/c - 1$ and $\Delta b/c = b/c - 1$ evaluate a variation of unit cell dimensions a and b (Fig. 1, b) reckoned from the corresponding values for

the crystalline Si, in which both those distances are equal to c. The relative surface deformations $\Delta b/c$ and $\Delta a/c$ were considered (see Fig. 1, b) along the dimer rows on the studied surface and in the direction perpendicular to them, i.e. along the bonds between the dimers, respectively. In the interval of elastic deformations, in accordance with the Hooke law, $\Delta a/c$ and $\Delta b/c$ are proportional to the corresponding stresses. The sign "−" or "+" before the magnitudes of $\Delta a/c$ and $\Delta b/c$ means that the stress is tensile or compressive, respectively. The changes of characteristic dimensions, $\Delta a/c$ and $\Delta b/c$, induced by the following factors were considered: (i) the formation of ad-dimers on the surface ($\Delta a_{ad}/c$ and $\Delta b_{ad}/c$), (ii) adsorption of O_2 molecules ($\Delta a_{O2}/c$ and $\Delta b_{O2}/c$), (iii) adsorption of one, two, or three O atoms ($\Delta a_O/c$ and $\Delta b_O/c$); and (iv) diffusion of a single O atom into the near-surface layers of the specimen ($\Delta a_d/c$ and $\Delta b_d/c$).

The energy values per unit cell calculated for various cell types (without O atoms, with an O_2 molecule, and with one to three O atoms) were compared with the use of the difference $\Delta E = E - E_0$. Here, E is the energy of the examined structure, and E_0 is the energy of the same structure in the most energetically favorable configuration. The comparison was made only for cells with the identical number of Ge atoms, because Ge atoms have more electrons than Si ones, so that the energy of a cell with Si atoms is lower than that, in which two Si atoms are substituted with Ge ones.

2.2. Substantiation of the approach chosen to analyze stresses

A method of surface stress calculation was described in the literature; it was successfully applied to the analysis of stresses in the systems Si(001)–2×1 and Si(001)–4×2 [12], as well as Sb/Si(001), Sb/Ge(001), and As/Si(001) [13–15]. The equilibrium positions of atoms in the unit cell and the translation vectors in the analyzed system were determined by minimizing the system energy. The position of atoms in the unit cell could change in all directions, but provided that the magnitudes of two translation vectors in the surface plane remained constant. These constant values were selected to equal the relevant values in crystalline Si. The positions of atoms in the unit cell and the length of the third translation vector directed perpendicularly to the surface were optimized until the corresponding diagonal component in the stress tensor vanished.

As was shown in work [16], O adatoms on the Ge_xSi_{1-x}/Si(001) surface shift the core levels $2p$ and $3d$ of those atoms at the surface which are located at a distance of about 4 Å from them. This fact points to a capability of oxygen to interact with the surface and change the positions of atoms at the distance that almost coincides with the magnitudes of translation vectors for the unit cell (5 Å). Hence, if the magnitudes of translation vectors are fixed, as it was done in works [12–15], it can induce substantial errors in the determination of system energies and, as a consequence, can result in an incorrect estimation of stresses. In this connection, we regard the calculation technique used in works [12–15] as not completely adequate for the determination of stresses at the initial stages of the Ge_xSi_{1-x}/Si(001) surface oxidation.

Within the Hooke law limits, the result of surface stress action is the variation of atomic positions on the surface. Therefore, the latter can be analyzed with the use of the relative variations in the characteristic unit cell dimensions, $\Delta a/c$ and $\Delta b/c$ (the relative deformations), which emerge under the action of ad-dimers on the surface and the adsorption of O atoms and oxygen molecules on them.

3. Results of Calculations and Their Discussion

3.1. Stresses at the Ge_xSi_{1-x}/Si(001) surface and the Ge_xSi_{1-x}/Si(001) surface with an adsorbed O_2 molecule

The most probable adsorption configurations for pure (Si–Si and Ge–Ge) and mixed (Si–Ge) ad-dimers on the Ge_xSi_{1-x}/Si(001) surface were found by us in

Table 1. **ΔE for structures in Fig. 2 and the corresponding variations of characteristic unit cell dimensions $\Delta a_{ad}/c$ and $\Delta b_{ad}/c$ after the dimer formation on the Ge_xSi_{1-x}/Si(001) and Si(001) (4 × 2) surfaces**

	$\Delta a_{ad}/c \times 10^{-2}$	$\Delta b_{ad}/c \times 10^{-2}$	ΔE
Ge–Ge (Fig. 2, a)	−0.71	2.67	0.0
Ge–Si (Fig. 2, b)	−0.75	3.12	0.96
Ge–Si (Fig. 2, c)	−0.74	3.12	1.02
Si–Si (Fig. 2, c)	−0.77	2.89	–
Si(001)(4 × 2)	−1.21	2.56	–

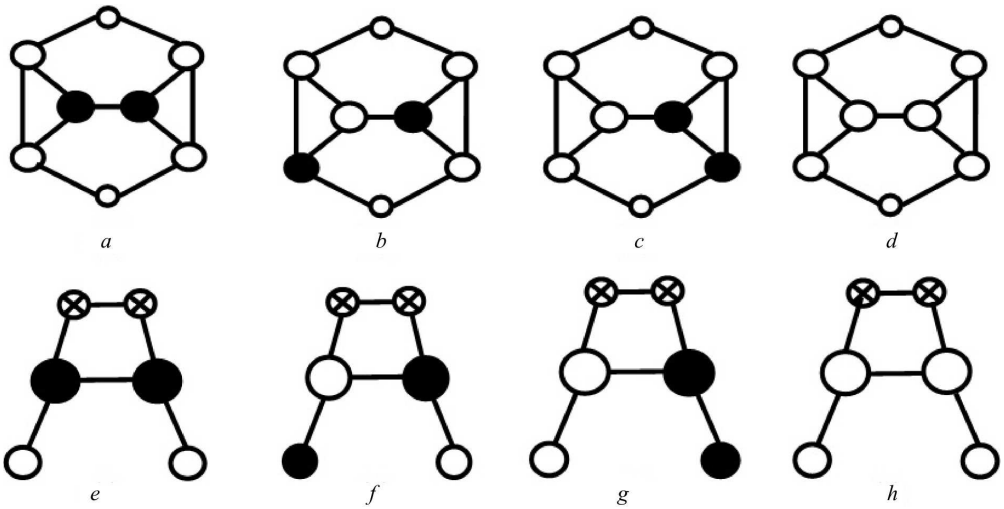

Fig. 2. Possible configurations of pure (Si–Si and Ge–Ge) and mixed (Si–Ge) ad-dimers on the Ge_xSi_{1-x}/Si(001) surface [17] (*a* to *d*) and the corresponding stable adsorption configurations with an adsorbed O_2 molecule [18] (*e* to *h*). Large and small black circles denote Ge and O atoms, respectively; and large and small hollow circles correspond to Si atoms in the second or third near-surface layer, respectively

work [17]. They are exhibited in Fig. 2 (panels *a* to *c*). The calculated values of ΔE, $\Delta a_{ad}/c$, and $\Delta b_{ad}/c$ for the Ge_xSi_{1-x}/Si(001) and Si(001)(4×2) surfaces with the most probable ad-dimer configurations for the structures depicted in Fig. 2 are quoted in Table 1. In analogy with the results of work [17], the configuration with pure Ge–Ge ad-dimers turned out the most beneficial energetically ($\Delta E = 0$) on the Ge_xSi_{1-x}/Si(001) surface.

The data in Table 1 show that there arise anisotropic ($\Delta a_{ad}/c \neq \Delta b_{ad}/c$) surface stresses on the surface of Ge_xSi_{1-x}/Si(001) systems with pure (Si–Si and Ge–Ge) and mixed (Si–Ge) ad-dimers: they are compressive ($\Delta b_{ad}/c > 0$) along the dimer rows and tensile ($\Delta a_{ad}/c < 0$) in the perpendicular direction (along the interdimer bonds). In the latter case, the stress magnitude is one third as large as in the former one. These data qualitatively agree with the experimental one obtained in work [19], where the stresses on the Si(001) surface with various coverage degrees (0 to 2 Ge monolayers) were studied.

In work [12], the stresses at the Si(001)(4×2) and Si(001)(2×1) surfaces were calculated. Only tensile surface stresses were revealed, both along the dimer rows and in the perpendicular direction, which does not coincide with our result. To elucidate the origin of this discrepancy, we carried out auxiliary calculations of surface stresses at the Si(001)(2×1) surface in the framework of our model with larger values of cut-off energy and a larger number of points when integrating over the Brillouin zone. The surface stresses were determined following the method described in works [12–15]. The data obtained are quoted in Table 2, with the signs "+" and "−" denoting the tensile and compressive stresses, respectively.

From Table 2, one can see that the cut-off energy increases from 136 eV (this value was taken in

Table 2. **Stresses along, σ_a, and perpendicularly to the dimer row, σ_p, on the Si(001)(2×1) surface reckoned in terms of eV/(1×1-cell) units and their anisotropy $\sigma_p - \sigma_a$ calculated according to the surface model [12] with various cut-off energies E and various number of k-points while integrating over the Brillouin zone: (*a*) $k = 6$ and $E = 136$ eV, (*b*) $k = 256$ and $E = 218$ eV, and (*c*) discretization of the Brillouin zone according to the Monkhorst–Pack scheme with the 2×1×1-grid and two layers of fixed atoms at the cell middle**

	σ_a	σ_p	$\sigma_a - \sigma_p$
a [12]	0.3	2.1	1.8
b	2.14	0.56	−1.58
c	−0.86	0.11	0.97
Experiment [20]	–	–	1

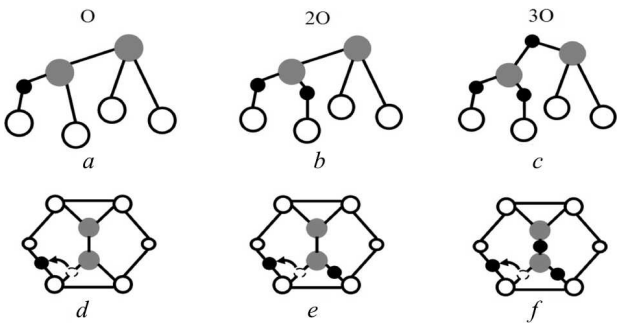

Fig. 3. Stable adsorption configurations of 1 (a), 2 (b), and 3 (c) O atoms and (d to e) the corresponding structures formed after a single O atom transits into the gap between the atoms in the second and third near-surface layers of Ge_xSi_{1-x}/Si(001). Grey and black circles denote Ge and O atoms, respectively; large and small hollow circles correspond to Si atoms in the second or third near-surface layer, respectively

work [12]) to 218 eV substantially changes the surface stresses (σ_a and σ_p). This result allows us to assert that the cut-off energy of 136 eV used in work [12] turned out insufficient for the surface stresses to be evaluated correctly. Moreover, the authors of work [12] used a cell in the form of a plate with 12 layers of Si atoms, with the top and bottom surfaces having undergone a 2×1-reconstruction, and the calculation model supposed a complete optimization of the atomic coordinates in the plate, which excluded the influence of the reconstruction in either part of the plate on its other part. In view of the literature data [21] testifying that the reconstruction of the Si(001) surface changes the position of atoms even in the eighth layer, it is possible to consider that a model neglecting the influence of a reconstruction in either of its part on the other part should give rise to wrong predictions. In this connection, we recalculated the surface stresses arising in this system with two fixed atomic layers in the middle (see row iii in Table 2) and found that the surface stresses became compressive along the dimer rows and remained tensile in the perpendicular direction. The anisotropy of those stresses was determined to equal $\sigma_p - \sigma_a = 0.97$ eV per 1×1-cell, which agrees with experimental data [20]. We also used this model to evaluate stresses at the reconstructed Si(001)(4×2) surface and also found that they became compressive ($\sigma_a < 0$) along the dimer rows and remained tensile ($\sigma_a < 0$) in the perpendicular direction (Table 2). All that allows us to assert that our model and the approximations made at calculations were adequate and made it possible the correctly evaluate the character of surface stresses in the examined systems.

Table 3. **ΔE_{O2}-values and the changes of the characteristic unit cell dimensions $\Delta a_{O2}/c$ and $\Delta b_{O2}/c$ for the structures in Fig. 1 (panels d to f) after the adsorption of an O_2 molecule on the Ge_xSi_{1-x}/Si(001) surface**

	$\Delta a_{O2}/c \times 10^{-2}$	$\Delta b_{O2}/c \times 10^{-2}$	ΔE_{O2}
Ge–Ge (Fig. 2, e)	−0.46	2.84	0.44
Ge–Si (Fig. 2, f)	−0.40	3.23	1.26
Ge–Si (Fig. 2, g)	−0.44	3.31	0.0
Si–Si (Fig. 2, h)	−0.47	2.60	–

In our previous work [18], we identified the adsorption prestates of an O_2 molecule, which are schematically depicted in Fig. 2 (panels d to g). The calculated values of the characteristic dimension variations $\Delta a_{O2}/c$ and $\Delta b_{O2}/c$ induced by the prestate formation and the relative energies ΔE_{O2} are listed in Table 3. A comparison of those data with the data for ad-dimers from Table 1 testifies that O_2 admolecules on pure (Si–Si and Ge–Ge) and mixed (Si–Ge) ad-dimers almost do not change the values of $\Delta a_{O2}/c$ and $\Delta b_{O2}/c$, as well as the surface anisotropy with respect to $\Delta a_{ad}/c$ and $\Delta b_{ad}/c$, but affect the ΔE_{O2}-values, with $\Delta E_{O2} = 0$ for mixed Si–Ge ad-dimers.

Hence, the adsorption of an O_2 molecule onto ad-dimers on the Ge_xSi_{1-x}/Si(001) surface keeps the character of stresses at the clean surface almost intact. The adsorption of an O_2 molecule onto the mixed Si–Ge ad-dimers in the configuration shown in Fig. 2, f turns out the most beneficial energetically, which coincides with the results of our previous work [18].

3.2. Stresses at the Ge_xSi_{1-x}/Si(001) surface with one, two, or three adsorbed O atoms

In our previous work [16], it was shown that, after the bond between the O atoms in the O_2 admolecule has been broken, new stable adsorption configurations composed of separate O atoms are formed on the studied surface. Those stable adsorption configurations for the cases of one, two, and three O adatoms on the Ge_xSi_{1-x}/Si(001) surface are depicted in Fig. 3 (panels a to c). At the initial stages of the Ge_xSi_{1-x}/Si(001) surface oxidation, some O

atoms can also diffuse into the near-surface layers [22]. The structures that are formed after one, two, or three O adatoms diffuse beneath the second near-surface layer of the specimen are exhibited in Fig. 3 (panels *d* to *f*, respectively). The arrow in every panel denotes the direction of this diffusion. The changes in the characteristic dimensions ($\Delta a_a/c$ and $\Delta b_a/c$) of a unit cell with O adatoms on the $Ge_xSi_{1-x}/Si(001)$ surface were calculated for all those structures. We also calculated the relative variations of the characteristic unit cell dimensions ($\Delta a_d/c$ and $\Delta b_d/c$) after an O atom diffuses into the gap between the atoms in the second and third near-surface layers in the cases of one, two, and three O atoms adsorbed on the analyzed surface. The results of calculations are presented in Table 4.

As one can see from Table 4, $\Delta a_a/c < 0$ and $\Delta b_a/c > 0$ for the $Ge_xSi_{1-x}/Si(001)$ surface with one to three O adatoms (Fig. 3, panels *a* to *c*, respectively). Since $\Delta a_a/c < \Delta b_a/c$, we may assert that the adsorption of up to three O atoms onto the surface almost does not change the character of stresses inherent to the clean $Ge_xSi_{1-x}/Si(001)$ surface. The values of quantities $\Delta a_d/c$ and $\Delta b_d/c$ quoted in Table 4 testify that the diffusion transition of a single O atom into the gap between the atoms in the second and third near-surface layers also does not change the character of stresses in the studied system in the cases of one, two, and three adsorbed O atoms (Fig. 3, panels *d* to *f*). Hence, the diffusion transition of an O atom schematically depicted in Fig. 3 does not stimulate the stress relaxation in the system, i.e. the diffusion of O atoms into the near-surface layers of the $Ge_xSi_{1-x}/Si(001)$ surface at the initial stages of its oxidation is not stimulated by the intrinsic stresses in the system. Moreover, it is worth noting that, as was shown earlier [22], this transition is also energetically unprofitable [22]. Therefore, we may suppose that the diffusion of O atoms into the near-surface layers of $Ge_xSi_{1-x}/Si(001)$ at the initial stages of oxidation may most probably be associated with the developed morphology of the surface.

Table 4. **Changes of the characteristic unit cell dimensions ($\Delta a_a/c$, $\Delta b_a/c$) and ($\Delta a_d/c$, $\Delta a_d/c$) for structures in Fig. 3 with an O adatom (panels *a* to *c*) after its diffusion into the near-surface region (panels *d* to *f*, respectively)**

	$\Delta a_a/c \times$ $\times 10^{-2}$	$\Delta b_a/c \times$ $\times 10^{-2}$	$\Delta a_d/c \times$ $\times 10^{-2}$	$\Delta b_d/c \times$ $\times 10^{-2}$
Ge–Ge (Fig. 2, *a*)				
O	−0.69	2.80	−0.61	3.45
2O	−0.69	2.80	−0.64	3.74
3O	−0.41	2.49	−0.49	4.66
Ge–Si (Fig. 2, *b*)				
O	−0.68	2.82	−0.23	3.34
2O	−0.68	2.82	−0.52	3.94
3O	−0.51	2.88	−0.27	3.18
Ge–Si (Fig. 2, *c*)				
O	−0.68	2.82	−0.58	3.61
2O	−0.68	2.82	−0.58	3.70
3O	−0.56	2.61	−0.51	4.50
Si–Si (Fig. 2, *d*)				
O	−0.73	2.73	−0.62	3.56
2O	−0.69	2.80	−0.54	3.74
3O	−0.48	2.50	−0.19	3.26

4. Conclusions

It is shown that the analysis of variations in the unit cell dimensions (the cell deformations $\Delta a/c$ and $\Delta b/c$) under the action of the atomic and molecular adsorption and diffusion–in particular, oxygen atoms and molecules–can be used to analyze the character of surface stress changes in the $Ge_xSi_{1-x}/Si(001)$ systems in the interval of elastic deformations. The anisotropy of surface stresses is revealed: the stress along the dimer rows on the $Ge_xSi_{1-x}/Si(001)$ surface turned out compressive and approximately three times as large as the tensile stress in the perpendicular direction. The surface stresses weakly depend on the action of oxygen adatoms or admolecules, because the adsorption of O_2 molecules or up to three O atoms on the $Ge_xSi_{1-x}/Si(001)$ surface almost does not affect the character of surface stresses. The diffusion of an oxygen atom into the gap between atoms in the second and third near-surface layers of the $Ge_xSi_{1-x}/Si(001)$ surface at the initial stages of its oxidation does not change the character of its surface stresses, i.e. does not stimulate the stress relaxation.

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Received 03.06.13.
Translated from Ukrainian by O.I. Voitenko

О.А. Гринчук, І.П. Коваль, М.Г. Находкин

ПОВЕРХНЕВІ НАПРУЖЕННЯ НА ПОЧАТКОВИХ ЕТАПАХ ОКИСЛЕННЯ Ge_xSi_{1-x}/Si(001)

Р е з ю м е

За допомогою аналізу змін розмірів елементарних комірок, яке відбувається внаслідок утворення на їх поверхнях димерів або адсорбції атомів і молекул, якісно розглянуто пружні напруження чистої поверхні Ge_xSi_{1-x}/Si(001) та на початкових етапах її окислення. Вони мають майже однаковий характер, як для чистої поверхні Ge_xSi_{1-x}/Si(001), так і після адсорбції на неї молекул O_2 або 1-го, 2-х та 3-х атомів O. Напруження виявились анізотропними: вздовж димерних рядів вони були стискаючими та приблизно у 3 рази більшими від розтягуючих напружень у напрямку, перпендикулярному до димерних рядів (вздовж димерного зв'язку).