

Stress relief from missing dimers on Bi/Si(001)

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Abstract

Based on first principles calculations, we studied the structural properties of group V elements P, As, Sb and Bi on the Si(001) surface. For one monolayer of the group V atoms on the Si(001) substrate, stress and stress anisotropy scaled almost linearly with atomic size, implying that the obvious source of surface stress was atomic size effect. We found that stress relief was responsible for the $(2 \times n)$ reconstruction of Sb and Bi on the Si(001) surface. Stress anisotropy could be tuned through zero and reversed in sign with n ranging from 10 to 5.

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1. Introduction

It is well known that As, Sb or Bi as a surfactant can mediate the epitaxial growth of Ge on Si(001) surfaces [1]. Bi forms nanowires self-assembly on Si(001) [2]. For clean or one monolayer of group V elements covering Si(001), the most prominent feature is the (2×1) reconstruction. It can be supposed intuitively that group V atoms will break Si–Si dimers, fill dangling bonds of Si(001) and form symmetric dimers in the (2×1) reconstruction. The dangling bonds of

group V atoms are filled with two electrons (lone pair). As a result of passivating effects of group V atoms, these surfaces should thus be highly stable. Surface atoms form dimers to reduce surface energy by filling dangling bonds, but at the expense of increasing strain energy due to bond distortion. Surface reconstruction introduces a surface stress anisotropy: the stress σ_{\parallel} along the dimer bond is tensile, i.e., surface atoms would like to be closer together along this direction than they are; the stress σ_{\perp} along the dimer row is consequently compressive (such as Sb/Si(001) 2×1) or at least less tensile (such as As/Si(001) 2×1). The stress anisotropy, $F = \sigma_{\parallel} - \sigma_{\perp}$, is predicted to cause morphological instability [3–6], resulting in antiphase domain boundaries in order to relieve

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the stress anisotropy for Sb on Si(001) [5], or a stripe-like structure with alternating stress domains [3].

Although all four systems share the same reconstruction mechanism, their surface morphologies differ. Scanning tunneling microscopy (STM) images [7] have shown that Sb/Si(001) is considerably less ordered than As/Si(001). The long range (2×1) order on Sb/Si(001) is broken up by a high density of defects—either vacancies or antiphase domain boundaries (APBs). The Sb/Si(001) surface shows a ($2 \times n$) pattern with ($n \approx 11$) in low energy electron diffraction (LEED) experiments when deposition temperature is increased to 750 °C [8]. LEED experiments reveal also that Bi atoms on Si(001) form a ($2 \times n$) reconstruction, with n ranging from 13 at temperatures around 400 K down to 5 at temperatures of 800 K and above [9]. A basic building block of the ($2 \times n$) structure is the Bi dimer: its unit cell contains ($n - 1$) Bi dimers with a space for one Bi dimer vacancy (DV), which forms vacancy lines (VLs). However, neither APBs nor VLs have been experimentally observed for As/Si(001), which has a perfect (2×1) reconstruction pattern.

In order to explore the mechanisms involved, we systematically studied the structural properties of group V atoms P, As, Sb and Bi on Si(001). Although P appears mainly as a dopant, we still include the P/Si(001) system in this investigation as a comparison. It is helpful to understand the stability of Bi or Sb line structures on Si(001), which usually leads to the formation of self-assembled nanowires [2,10]. Since surface stress resulting from lattice mismatch in heteroepitaxial growth has often been thought to be responsible for nanoscale roughness and self-assembly of nanoscale features, we paid more attention to the surface stress of group V atoms on the Si(001) surface. Meade and Vanderbilt found that the surface stress plays an important role in determining the surface reconstruction and there are three microscopic origins of surface stress: the relative atomic sizes of the adsorbate and substrate atoms, the chemical nature of the adsorbate species, and the bonding topology of the surface reconstruction [6]. Based on first-principles calculations, we found that stress relief is the main driving force of ($2 \times n$)

reconstruction for Bi or Sb on the Si(001) surface, and the stress anisotropy can be tuned to zero and reversed in sign with n ranging from 10 to 5.

2. Methods

The first-principles calculations were performed using the VASP code under the framework of local density functional theory [11]. The wavefunctions are expanded in a plane-wave basis set, the electron-ion interaction is described by ultrasoft pseudopotentials. We use the generalized gradient approximation (GGA) for the exchange–correlation functional. The V–Si(001) surface is modeled as a repeated slab by taking a periodic arrangement. The calculated lattice-constant was 5.46 Å, in excellent agreement with that obtained by experiments, 5.41 Å. The k -point (32 points in the SBZ), slab thickness (14 layers), energy cutoff (188 eV) and vacuum spacing (27 Å) were chosen to ensure convergence to 0.04 eV for surface energy. Only the atoms in the two center layers are fixed, all coordinates of the adatoms and substrate atoms relaxed until their forces smaller than 0.01 eV/Å.

By definition, the surface stress tensor is given by

$$\sigma_{ij} = A^{-1} \frac{\partial(A\gamma)}{\partial \varepsilon_{ij}}, \quad (1)$$

where A is the surface area, $A\gamma$ the surface free energy, and ε_{ij} the two-dimensional external strain tensor. To estimate the surface stress, we use the relation [12,13]

$$\sigma_{ij}^{\text{surf}} = \frac{1}{2}c\sigma_{ij}^{\text{corr}} = \frac{1}{2}c(\sigma_{ij}^{\text{bulk}} + \chi\delta_{ij}). \quad (2)$$

where $\sigma_{ij}^{\text{bulk}}$ is the three-dimensional supercell stress tensor, c is the height of the supercell, and χ is a basis set correction to the diagonal elements of the supercell stress tensor. This basis-set correction occurs because the plane-wave (PW) basis set is not complete with respect to changes of the volume. This error is often called “Pulay stress” [14] and is almost isotropic (i.e. the same for each diagonal component). In our calculations, the choice of $\chi = -\sigma_{zz}^{\text{bulk}}$ is used to satisfy the physical requirement of null z stress in the fully relaxed slab

[6,12]. Since the correction is same for each diagonal component, it will cancel when the stress anisotropy is calculated, and thus the stress anisotropy is considerably precise. Our tests show that the energy converges at 150 eV energy cutoff, and the stress converges at 188 eV energy cutoff. At 188 eV energy cutoff, the error bars for the diagonal components are around 0.1 eV/(1 × cell).

3. Results and discussions

3.1. (2 × 1) reconstruction

We use the (2 × 1) reconstruction as a starting point to investigate structural properties of the group V atoms on Si(001). A schematic top view is shown in Fig. 1(a). Based on the (2 × 1) symmetry, relaxed atomic structures were obtained for all four systems. In the calculations all atoms were fully relaxed until forces on atoms became smaller than 0.01 eV/Å. As expected, the adsorption atoms formed symmetric dimers on the Si(001) substrate without tilted angle. The calculated lengths of dimer bond and backbond are presented in Tables 1 and 2, respectively, in comparison with other results either predicted by calculations or measured by experiments.

The lengths of the dimer bond and backbond increased linearly with the Pauling radii in going from P to Bi. We found that phosphorus has the shortest dimer length, 2.31 Å, and its backbond length to subsurface Si was 2.38 Å, both were a little longer than the result that Gay et al. [15] obtained by using first-principles LDA calculation, 2.28 or 2.25 Å. Arsenic has a dimer length of 2.58 Å, in good agreement with the XSW experiment [16]. This dimer length is also remarkably close to the results result Cho and Kang [17] previously obtained using first principles LDA calculations. The calculated length of As–Si backbond was 2.46 Å, also in good agreement with that obtained by Cho and Kang [17]. Sb on Si(001) showed a dimer length of 2.97 Å and a backbond length of 2.59 Å, both of which appeared remarkably close to that obtained by other calculations (Tables 1 and 2). However, experiments suggested

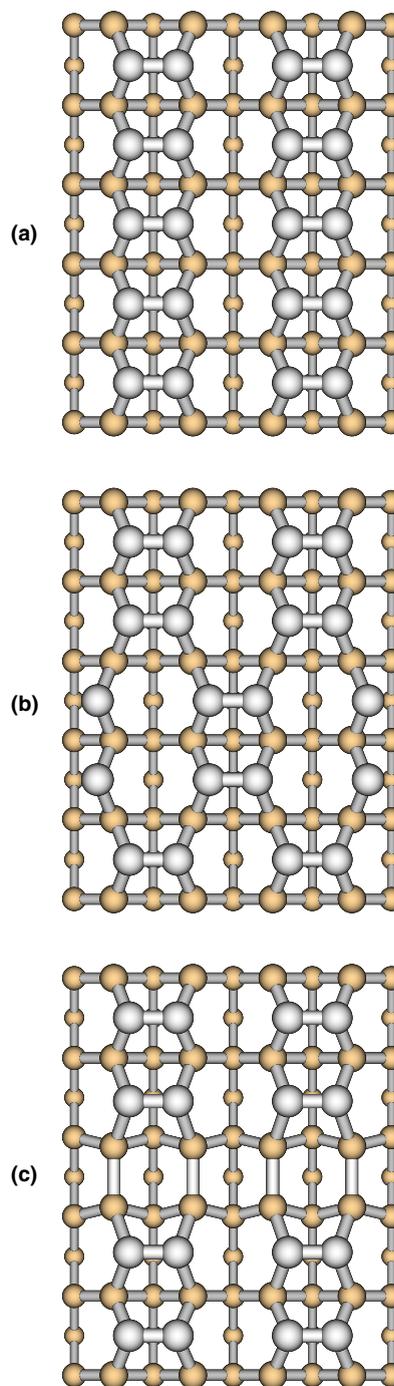


Fig. 1. Top view of (a) (2 × 1) reconstruction, (b) (2 × 4) reconstruction with the formation of APBs, and (c) (2 × 5) reconstruction with the formation of VLs.

Table 1
The dimer-bond lengths (in Å) for (2 × 1) group V overlayers on Si(001)

	P	As	Sb	Bi
<i>Theory</i>				
GGA (this work)	2.31	2.58	2.97	3.14
LDA [15]	2.28	2.51	2.96	3.06
LDA [17]	–	2.57	2.94	–
Semiempirical [5]	–	2.47	2.93	–
Dmol [19]	–	–	–	3.16
Pauling radius	2.21	2.50	2.90	3.10
<i>Experiment</i>				
XSW [19]	–	–	–	2.94 ± 0.06
XSW [18]	–	–	2.81 ± 0.09	–
XSW [16]	–	2.58 ± 0.04	–	–
SEXAFS [7]	–	–	2.88 ± 0.03	–

Table 2
The backbond lengths (in Å) for (2 × 1) group V overlayers on Si(001)

	P	As	Sb	Bi
<i>Theory</i>				
GGA (this work)	2.38	2.46	2.59	2.66
LDA [15]	2.25	2.42	2.56	2.62
LDA [17]	–	2.45	2.59	–
Semiempirical [5]	–	2.42	2.59	–
Dmol [19]	–	–	–	2.68
Pauling radius	2.28	2.42	2.63	2.72

a shorter dimer length, 2.81 ± 0.09 Å for Sb/Si(001) [18]. The dimer length for the Bi overlayer was 3.14 Å, in good agreement with that obtained by Franklin et al. [19] using the Dmol method, while the XSW technique yields a considerably smaller dimer length of 2.94 ± 0.06 Å. The Bi–Si backbond has a length of 2.66 Å, quite close to that obtained by Franklin et al. [19]. For all four systems, the dimer length is considerably close to that estimated by using Pauling radii, suggesting that group V atoms on Si(001) preserve their atomic properties after adsorption on Si(001). It can be thus concluded that the fundamental bonding mechanisms are identical.

In reality, the long-range ordered (2 × 1) reconstruction was observed for only As on Si(001). It was shown experimentally that there were APBs and VLs on Sb/Si(001) and Bi/Si(001), giving rise to the (2 × *n*) reconstruction for the both systems [2,7–10]. Since surface stress plays an important role in surface structure, we then calculated surface

stress for these systems. The calculated surface stresses for all four systems are listed in Table 3. The stress along the dimer bond for all four systems was positive, that is, σ_{\parallel} was tensile, reflecting that elastic reaction of backbonds opposed the dimerization and that the surface would like to shrink along the dimer bond in order to minimize backbond bending [20]. As expected, with increasing overlayer atomic number the tensile stress along the dimer bond decreased, since σ_{\parallel} was mainly caused by backbond bending which became less with increasing atomic size of overlayer.

However, the stress along the dimer row is somewhat complex. The group V atoms have a different atom size for P, As, Sb and Bi (atomic radii of 1.105, 1.248, 1.45 and 1.548 Å) compared to Si (1.176 Å). Therefore, a significant structural distortion and strain on the group V covered Si(001) can be expected. In order to understand the stress along dimer row for the group V atoms on Si(001), we used As to analyze the effect of the

Table 3

The surface stresses (in eV/(1 × 1 cell)) for (2 × 1) group V overlayers on Si(001)

System	σ_{\parallel}	σ_{\perp}	$(\sigma_{\parallel} + \sigma_{\perp})/2$	$F = \sigma_{\parallel} - \sigma_{\perp}$
P/Si(001) 2 × 1	2.3	2.9	2.6	-0.6
As/Si(001) 2 × 1	1.7	1.5	1.6	0.2
Sb/Si(001) 2 × 1	1.2	-1.5	-0.2	2.7
Bi/Si(001) 2 × 1	1.0	-2.6	-0.8	3.6

The symbol \parallel and \perp refer to the dimer-bond and dimer-row directions, respectively.

atomic size and chemical nature on stress, since the atomic radii of As (1.248 Å) is quite close to that of Si (1.176 Å). Arsenic has five valence electrons. Two participate in bonds to subsurface Si atoms and one to the other arsenic in the dimer, leaving two electrons to form the so-called lone pair in the dangling bond. Due to Coulomb repulsion between the lone pair and backbond charge, the remaining bonds of As prefer to a p^3 -like hybrid, that is, with an angle between backbonds less than those of a perfect tetrahedron. We found that the angle between two backbonds of As with Si atoms was 103.4°, less than 109.5° of an ideal sp^3 hybrid. However, this angle change was prevented by the 2 × 1 symmetry. Therefore, the As–Si bonds were stretched to satisfy the requirement for the angle change. A tensile stress could be expected for As on Si(001) along the dimer row. When As was replaced by the other group V atoms with smaller radii, the stress was more tensile, however, a larger atom reduced the tensile stress and even reserved it in sign to compressive. Since the atomic radii of P (1.105 Å) is smaller than that of As (1.248 Å), a more tensile stress along the dimer row can be obtained, while the atomic radii of Sb (1.45 Å) and Bi (1.548 Å) is much larger, a significant compressive stress was thus observed. The calculated angles between backbonds for P, As, Sb and Bi in dimer on Si(001) were 108.0°, 103.4°, 96.1° and 92.8°, respectively. The larger the atom, the smaller the angle between backbonds. We observed two contributions to the stress along the dimer row, atomic size effect and rehybridization effect. That is, the resulting stress in these cases depended not only on atomic size but also on chemical nature. With increasing atomic size, the stress along the dimer row for group V atoms on Si(001) decreased and might reverse in sign to compressive.

An increase of atomic size of the overlayer from P to Bi led to an increase of the stress in the direction of dimer rows, and a decrease of the stress in the direction of dimer bonds. Thus the stress anisotropy increased with increasing atomic size of the overlayer. Fig. 2 shows the relationship between atomic size and stress anisotropy as well as the stress along two directions. The stress and stress anisotropy scale almost linearly with atomic size.

This conclusion was obtained based on the calculations under an assumption of the (2 × 1) reconstruction without APBs or VLs formation. The P and As overlayer systems formed a similar pair in regards to the calculated surface stresses, that is, the stress along the dimer row was tensile, and the Sb and Bi systems formed another similar pair, that is, the stress along the same direction was compressive. Therefore, the systems of Sb and Bi

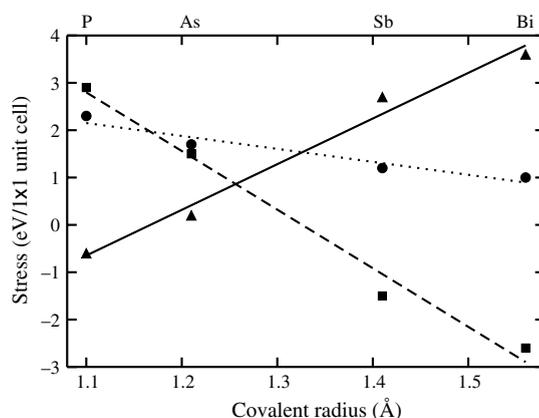


Fig. 2. Surface stress vs. the Pauling radius for (2 × 1) group V overlayers on Si(001). The solid line represents stress anisotropy, the dotted line represents surface stress along the dimer bond, and the dashed line represents surface stress along the dimer row.

on Si(001) suffered a large stress anisotropy and were unstable. In order to decrease the stress anisotropy and relieve the compressive stress along the dimer row, the long-range (2×1) symmetry for these systems should be broken. Since intricate interplay existed between surface stress and surface morphology, it was suggested that the relief of surface stress might provide a mechanism to create an ordered array of surface defects, that is, antiphase boundaries (APBs) and missing dimers (or dimer vacancies, DVs) in a ($2 \times n$) structure [3–5,21]. Despite the fact that APBs and DVs usually intermix each other to form the ($2 \times n$) reconstruction on Bi- or Sb-covered Si(001), we investigated the formation of APBs and DVs separately.

3.2. ($2 \times n$) reconstruction

In order to check whether stress relief is responsible for the formation of the $2 \times n$ reconstruction on Bi/Si(001), we introduced a (2×4) reconstruction, obtained by shifting two dimers to a trench between dimer rows, as Fig. 1(b) depicts. An essential APBs feature is that no symmetric restriction exists in the direction of dimer row compared with the (2×1) reconstruction because one part of a dimer row has been shifted to the nearest trench. For comparison, we also give the results for Sb/Si(001). For the (2×4) surface unit cell, 8 k -points for the Brillouin-zone sampling were used, and the other setups were the same as the (2×1) reconstruction above.

The calculated results for stress are listed in Table 4. It was shown that the defect relieved a compressive stress with a value of 0.2 eV/(1×1 cell) along the dimer row both for Sb and Bi on Si(001). The APBs do not change the stress along

the dimer bond. This finding was quite close to the semiempirical result for Sb/Si(001) (about 0.3 eV/(1×1 cell)) [5]. The greatest displacement of Sb atoms in the direction perpendicular to dimer is only 0.01 Å. This displacement was due to breaking the symmetric restriction, leading to relieving the compressive stress along the dimer row [5]. However, in contrast to the case of Sb/Si(001), the formation of APBs on Bi/Si(001) relieved only a small part of the stress anisotropy (around 10%).

We then check the influence of DV formation on stress. Since it was shown experimentally that for Bi/Si(001) the n can reach a value of 5 at temperatures of 800 K and above [9], we first considered a (2×5) surface unit cell (with one DV per four dimers) for both Sb/Si(001) and Bi/Si(001) (see Fig. 1(c)). For the (2×5) surface unit cell, we use 8 k -points for the Brillouin-zone sampling in calculations, and the other setups were the same as those the (2×1).

The calculated results are listed in Table 4. For Sb–Si(001) 2×5 , the surface stress changed little (only 0.2 eV/(1×1 cell)) along the dimer bond and greatly (3.9 eV/(1×1 cell)) along the dimer row. For Bi–Si(001) 2×5 , the surface stress also changed little (only 0.1 eV/(1×1 cell)) along the dimer bond and greatly (4.3 eV/(1×1 cell)) along the dimer row. The surface stress along the dimer row reversed in sign. The missing dimers left a space for dimers beside the dimer vacancy (DV). Thus, two dimers beside the DV were closer to each other and relaxed to the DV along the dimer row, about 0.54 Å for Sb–Si(001) 2×5 and 0.59 Å for Bi–Si(001) 2×5 . Further relaxation of the other two dimers was induced towards the DV about 0.14 Å for Sb–Si(001) 2×5 and 0.15 Å for Bi–Si(001) 2×5 , indicating that the missing dimers provided a space for the expansion of the Sb or Bi

Table 4

The surface stresses (in eV/(1×1 cell)) for ($2 \times n$) reconstructions of Sb and Bi on Si(001)

System	σ_{\parallel}	σ_{\perp}	$(\sigma_{\parallel} + \sigma_{\perp})/2$	$F = \sigma_{\parallel} - \sigma_{\perp}$
Sb/Si(001) 2×4 (APBs)	1.2	–1.3	–0.1	2.5
Sb/Si(001) 2×5 (VLs)	1.0	2.4	1.7	–1.2
Bi/Si(001) 2×4 (APBs)	1.0	–2.4	–0.7	3.4
Bi/Si(001) 2×5 (VLs)	0.9	1.7	1.3	–0.8

The symbol \parallel and \perp refer to the dimer-bond and dimer-row directions, respectively.

layer and relieved the compressive stress along the dimer row.

Simply removing a dimer will create two extra dangling bonds in the second layer, at the cost of raising strain energy. Pandey [22] proposed that by removing a dimer and then rebonding the second-layer atoms, the number of dangling bonds could be reduced, albeit at a considerable cost in local strain. According to our calculations, when a dimer was removed, the Si atoms underneath were pulled together and rebonded along the dimer row. The distance between the rebonded atoms is 2.60 Å for Sb–Si(001) 2×5 and 2.53 Å for Bi–Si(001) 2×5 . Compared to the length of Si dimer on clean Si(001), 2.31 Å, the bond length would like to be shorter. However, the substrate prevented the shortening. Therefore, it could be concluded that the rebonding Si atoms under the DV led to tensile stress along the dimer row due to the restriction of the substrate. This tensile part induced by the rebonding Si atoms under the DV compensated for the compressive stress along the dimer row induced by hybridization of Sb or Bi in dimer. This relief of the stress along dimer row was derived from the expansion due to the space left by the missing dimers in the first layer (i.e., relieving the compressive stress), and from the tensile stress due to rebonding of the dangling bonds in the subsurface under the DV (compensates for a part of the compressive stress).

According to the discussion above, two competing factors for stress relief are the compressive and tensile contribution. A preferred spacing, na_0 , should exist between two neighboring DVs on the same dimer row. If they are too far apart, the compressive stress is not relieved enough; if they are too close, the stress is *over-relieved*. Effectively, the balancing of tensile and compressive stresses amounts to a short-range repulsive and a long-range attractive interaction between DVs on the same dimer row, as shown directly by total energy calculations on Ge/Si(001) [4,23]. The value of the factor n on Bi–Si(001) ranges from 13 to 5 with elevated temperatures [9], corresponding to a coverage $\theta = 1 - 1/n$. Fig. 3 shows the surface stress of Sb- or Bi-Si(001) $2 \times n$ vs. θ . The point for $\theta = 1$ corresponds to the ideal 2×1 structure. All these calculated structures correspond to θ chang-

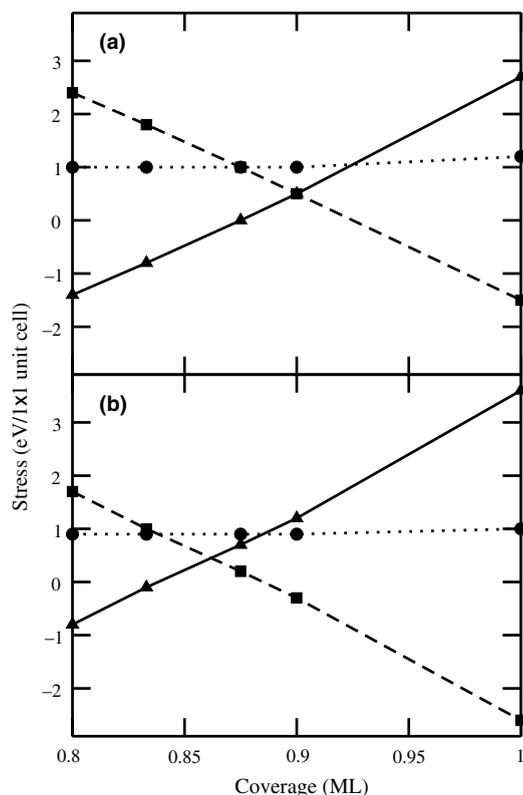


Fig. 3. Surface stress vs. coverage for (a) Sb- and (b) Bi-covered Si(001) from the first-principles calculations. The solid line represents stress anisotropy, the dotted line represents surface stress along the dimer bond, and the dashed line represents surface stress along the dimer row.

ing from 0.8 to 1. Our data are similar with those of Ge/Si(001) [4,23]: σ_{\parallel} is essentially unchanged, while with decreasing $n\sigma_{\perp}$ increases, i.e., the σ_{\perp} becomes more tensile. Since the rebonding of atoms in the subsurface is in a direction perpendicular to the dimer bond, increasing n mainly modifies σ_{\perp} while leaving σ_{\parallel} unchanged.

Interestingly, the stress and anisotropy scaled almost linearly with coverage. We found that σ_{\perp} almost equals zero at $n \approx 10$ for Sb–Si(001) and $n \approx 8$ for Bi–Si(001), the zero surface-stress anisotropy is estimated at $n \approx 8$ for Sb–Si(001) and $n \approx 6$ for Bi–Si(001). The $(2 \times n)$ reconstruction was expected to be the most favorable one at $n \approx 10$ for Sb–Si(001) and at $n \approx 8$ for Bi–Si(001), since the average stress $(\sigma_{\parallel} + \sigma_{\perp})/2$ reached the minimum and the compressive strain

energy was relieved. σ_{\perp} was *over-relieved* at $n = 5$ and reversed in sign of the stress. Then, σ_{\perp} was even more tensile than σ_{\parallel} . Thus the (2×5) reconstruction should be unfavorable. For Sb–Si(001), the Si atoms under the DV rebonded along the dimer row, the distance was 2.60, 2.58, 2.56 and 2.56 Å at $n = 5, 6, 8$ and 10, respectively. For Bi–Si(001), these values were 2.53, 2.52, 2.50 and 2.50 Å at $n = 5, 6, 8$ and 10, respectively. The distance of the rebonded subsurface Si atoms was almost constant with n , and changes smaller than 0.04 Å for Sb and Bi. Therefore, the distance of the rebonded Si atoms was mainly controlled by the structure, leading to a tensile stress as discussed above. For Sb–Si(001), the dimers beside the DV were pulled towards the DV about 0.54, 0.57, 0.60 and 0.61 Å at $n = 5, 6, 8$ and 10, respectively, and for Bi–Si(001), these values read 0.59, 0.62, 0.65 and 0.66 Å at $n = 5, 6, 8$ and 10, respectively. Based on previous discussions, the $(2 \times n)$ reconstruction must not exist on As- and P-Si(001), since the both systems were tensile-stressed along the dimer row. The creation of periodic vacancy lines made σ_{\perp} more tensile and increased the anisotropy. We obtained $\sigma_{\parallel} = 1.4$ eV/(1 × 1 cell) and $\sigma_{\perp} = 3.5$ eV/(1 × 1 cell) from the calculation of As–Si(001) 2×5 . It is obvious that the As–Si(001) 2×5 is not a stable structure.

An interesting feature in DVs observed by experiments was an ordering of DV in a direction perpendicular to the dimer row: DVs on the different dimer rows are aligned each other to form the so-called vacancy line (VL). The microscopic origin of this ordering should be similar with that of Ge/Si(001) [4,24]. We thus carried out total-energy calculations for interaction between DVs. In the calculations we used a 4×5 unit cell, which contained two missing dimers (see Fig. 1(c)). To obtain the interaction energy of the DVs on the adjacent dimer rows, we move the adjacent DV by a_0 , and relax all atoms. The zero separation between the DVs on the neighboring dimer rows was found to have the lowest energy. When the separation was one lattice constant, the energy became 0.13 and 0.15 eV/DV higher compared to the zero separation for Sb and Bi on Si(001), respectively, while their surface stresses had no significant changes for the both systems (smaller than 0.1

eV/(1 × 1 cell)). The present total-energy calculations clearly showed an attractive interaction exists between the DVs on the adjacent dimer rows. The DVs aligned straight in a direction perpendicular to the dimer row were more stable. Most importantly, this attractive interaction explained the appearance of the domain of the width na_0 separated by the VLs. Furthermore, our calculations revealed another interesting physical mechanism: the stability of VLs varies with atomic size, meaning that a larger atomic size might make VLs more stable.

4. Conclusions

In summary, we studied the morphologies and surface stresses of group V overlayers on the Si(001) surface. It was shown that upon adsorption on the Si(001) substrate the group V atoms form symmetric dimers. For the (2×1) geometry, the stress and anisotropy scaled almost linearly with atomic size, reflecting that the most obvious source of surface stress is an atomic size effect. The calculations of surface stress variations confirm that the stress relief is responsible for the $(2 \times n)$ reconstruction. The driving forces generated by the surface stress and its anisotropy introduce significant changes in surface morphology. The results show that the stress and anisotropy scale linearly with coverage. The stress anisotropy can be tuned through zero and reversed in sign with n ranging from 10 to 5. The DVs tend to align in a straight line perpendicular to the dimer row.

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