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Full Length Article

Study of atomic arrangements and charge distribution on Si(0 0 1) surfaces with the adsorption of one Ge atom by DFTB calculations

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ABSTRACT

Density Functional Tight Binding (DFTB) calculations are performed to study atomic arrangements and charge distribution of Si(0 0 1) surfaces with one Ge atom adsorbate. For these Ge/Si(0 0 1) systems, the initial height between the Ge atom and the surface, and the adsorption position being relative to the Si dimers on the surfaces, have influences on the stable structures of the Ge atom on the Si surface. Firstly, two reconstructed Si(0 0 1) surfaces including c(4 $\times$ 2) and p(2 $\times$ 2) are obtained. Then, the Ge atom is placed on these two reconstructed surfaces. The calculations show the following results. For these dimers formed on the two Si(0 0 1) surfaces, dimer's bond length, and the buckling angle between the dimer and the surface have apparent differences as well as the charge distribution of these two surfaces. The Ge atom prefers to be located at two positions of the dimer: the outside top position of one atom of the dimer and the bridge position of this dimer. In these systems, the Ge atom always loses charges, and the charge transfer is found between atoms of one Si dimer. The asymmetric deviation of the two atoms in the dimer greatly affects the structure and charge distribution of Ge atom and the dimer.

1. Introduction

SiGe/Si heterogeneous materials have been widely used in microelectronics and optoelectronic devices. Preparation of precise and controllable SiGe/Si heterogeneous nanometer materials increases the performance of electronic devices [1–5]. Li et al.'s studies show that ultra-thin layers or monolayer Si/Ge films can improve the high responsivity of the vertical-illumination Si/Ge uni-traveling carrier (UTC) devices because of nanoscale effect [1]. In the process of epitaxial growth to prepare SiGe/Si heterogeneous materials, the adsorption of Ge atoms on the surface of Si substrate is the first step of the growth. When Ge atoms are adsorbed on Si(0 0 1) surface, the changes of the Si(0 0 1) surface can be observed both in experiments [6,7] and theoretical calculations [8–12]. Krüger et al. found that the Si substrate surface presents metallic properties as the Ge atoms were adsorbed on special positions of the Si substrate [8]. Therefore, one of the key problems is arisen on how to control sedimentary position of Ge atoms on Si substrates in the epitaxial growth process.

In laboratory, atom rearrangements on the Si substrate surface occur, and the reconstructed surface plays an important role in forming SiGe/Si films by epitaxial growth technology [13–15]. Here, the c(4 $\times$ 2) and p(2 $\times$ 2) reconstructed surfaces of the Si(0 0 1) substrates have been observed both in experimental and theoretical studies [16,17]. Therefore, the adsorption positions as well as surface structures of the substrate greatly affect the structures and properties of the substrate surfaces in the process of the heterogeneous epitaxial growth.

In this paper, Density Functional Tight Binding (DFTB) simulations are performed to study the effect of some possible adsorption positions on the structure stability and charge distribution for the systems of the adsorbed Ge atom on the Si(0 0 1) surfaces, where the Si(0 0 1) surfaces with asymmetric dimers present the c(4 $\times$ 2) and p(2 $\times$ 2) patterns.

2. Computational details

The source code and Slater-Koster files including Si-Si, Ge-Ge, Si-Ge, and Ge-Si are provided by Dr. Yi Dong and Professor Michael Springborg of University of Saarland in Germany. These codes and S-K files have been used to describe the infinite, periodic, and

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crystalline systems. Using these S-K files, the optimized lattice constants of crystalline Si and Ge are 5.46 and 5.71 Å respectively, which are less than 1% of the experimental values [18,19]. In our calculations, the energy threshold value is set to 0.0002 eV. When the difference between the energy values of the present step and the previous step is less than this threshold value, the calculations stop. If this constraint condition is not satisfied, each calculation runs 3000 steps.

Initially, in order to obtain different surface structures which was observed in experiments, two diamond Si(0 0 1) slabs are periodically built with 3 × 3 and 6 × 6 unit cells along [1 0 0] and [0 1 0] directions respectively, and there are 3 atomic layers (about 0.272-nm-thickness) along the [0 0 1] direction, as shown in Fig. 1(a)-(d). A vacuum gap with the width of 265.00 Å is introduced between the slabs. Here, the lattice constant a_0 of Si bulk is 5.43 Å. In these figures, green balls represent the bottom layer corresponding to the lower surface, orange pink balls the middle layer, and purple balls the top layer corresponding to the upper surface. Fig. 1(a) and (c) are top views along the [0 0 1] direction of these two Si slabs, and the side views are shown in Fig. 1(b) and (d) along the [0 0 1] and [1 1 0] directions. Then, DFTB algorithm is used to obtain reconstructed surfaces of these built surfaces. After obtaining these surfaces, one Ge atom is placed on these reconstructed Si(0 0 1) surfaces with different positions.

When the epitaxial Ge atom adsorbed on the Si(0 0 1) surface, the adsorption energy is:

$$E_{ads}(Ge/Si_{slab}) = E_{tot}(Si_{slab}) + E(Ge) - E_{tot}(Ge/Si_{slab}), \quad (1)$$

where E_{tot} is the total energy of the calculated system, E_{ads} the adsorption energy, and. E(Ge) the energy of Ge single atom, which is the energy sum of s and p orbits provided in the S-K file for Ge-Ge.

The surface energy can be calculated from the following equation,

$$\gamma = \frac{E_{slab} - N \cdot E_{bulk}}{2A} \quad (2)$$

where E_{slab} is the total energy of surface slab, N is the number of atoms in this slab, E_{bulk} is the energy per atom in bulk phase, and A is the surface area.

3. Results and discussions

3.1. Reconstructed Si(0 0 1) surface

Figs. 2 and 3 show different patterns of the reconstructed Si(0 0 1) surfaces with 3 × 3 and 6 × 6 unit cells. As shown the top views of these two Si slabs along the [0 0 1] direction in Figs. 2 and 3 (a), the atoms in the top layer move close to each other along the [1 1 0] direction, and these atoms alternately form dimers having "Zigzag" patterns. Meanwhile, some of these atoms in these dimers present upward movements along the [0 0 1] direction as shown the side views along the [0 0 1] and [1 1 0] directions, whereas the others downward movements. Figs. 2 and 3(b) show the buckling on the surfaces, where the dimers on the upper surface present different patterns. As shown in Figs. 2 and 3(c), along the [−1 1 0] direction, the two atoms in one dimer are upward and downward respectively from the surface. For the case of the 3 × 3 unit cells, the plaid purple balls represent the upward atoms from the surface, and the other purple balls the downward atoms from the surface. As observed along the [−1 1 0] direction, for the two interval dimer columns being connected with solid lines, including dimer_1 to dimer_4, their buckling direction is consistent with each other, and the similar picture also appears for the two interval dimer rows connected with solid lines along the [1 1 0] direction. Therefore, the p(2 × 2) reconstruction pattern is formed for the 3 × 3 unit cells in the Si slab [17]. For the surface atoms of the 6 × 6 unit cells in the Si slab, the formed dimers have the same buckling direction, which are connected with solid lines from dimer_1 to dimer_4 as shown in Fig. 3(c). The reconstructed surface presents c(4 × 2) pattern having opposite buckling dimers with intervals [16]. Figs. 2 and 3(d) respectively show the regions marked by dots

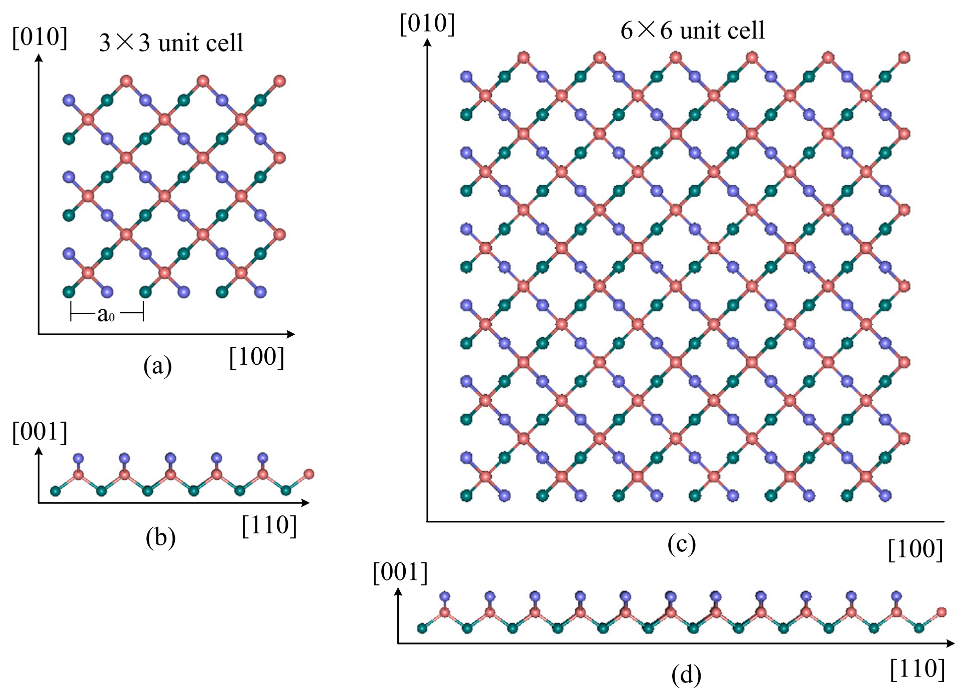

Fig. 1. Constructed Si(0 0 1) surfaces of a 3-layer slab with 3 × 3 unit cells and 6 × 6 unit cells along [1 0 0] and [0 1 0] directions; (a) top view along the [0 0 1] direction of 3 × 3 unit cells; (b) side view along [0 0 1] and [1 1 0] directions of (a); (c) top view of 6 × 6 unit cells; (d) side view of (c), where green balls represent the bottom layer corresponding to the lower surface, orange pink balls the middle layer, and purple balls the top layer corresponding to the upper surface. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)