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Surface Science 600 (2006) 1107–1112
SURFACE SCIENCE
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Ge adsorption on SiC(0001): An ab initio study

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Received 14 September 2005; accepted for publication 22 December 2005
Available online 26 January 2006

Abstract

In this work we have performed an ab initio total energy investigation of the Ge adsorption process on the Si-terminated SiC(0001)-$(\sqrt{3}\times\sqrt{3})R30^{\circ}$ and (3×3) surfaces. We find that Ge adatoms lying on the topmost sites of the $(\sqrt{3}\times\sqrt{3})R30^{\circ}$ and (3×3) surfaces represent the energetically more stable configurations at the initial stage of the Ge adsorption on the SiC(0001) surface. The Si → Ge substitutional adsorption processes have been examined as a function of the Si and Ge chemical potentials. Increasing the Ge coverage, we verify that the formation of Ge wetting layer on the $(\sqrt{3}\times\sqrt{3})R30^{\circ}$ surface, and Ge nanocluster on the (3×3) surface are the energetically more stable configurations, in accordance with recent experimental findings.
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Keywords: Density functional theory; Adsorption; Growth process; SiC; Ge and Si

1. Introduction

Semiconductor surfaces play an important role to the development of new electronic and optoelectronic devices. Due to its technological appeal, silicon surfaces have been the most studied ones. However, in the past few years, silicon carbide (SiC) has attracted numerous experimental and theoretical works. SiC has unique properties like high temperature stability, low weight, and high strength. Those properties make SiC a very promising material for new electronic and biological devices. It is clear that the development of those devices are closely related to the understanding of the chemical interactions between SiC surfaces and external atoms or molecules. For instance, the interaction of water with the SiC(001) surface [1,2], the adsorption of group III atoms on SiC(0001) surfaces [3], and the oxidation process of 6H–SiC(0001)-(3×3) [4,5]. Further experimental investigations verified the formation of Ge-nanocrystals in SiC (host material) by ion implantation [6,7], as well as the formation of Ge-nanoclusters through Ge adsorption process on SiC(0001) surfaces [8,9]. Those Ge nanoclusters open up the possibility of design self-assembled atomic arrangements with suitable electronic and structural properties. The Ge nucleation dynamics is closely related to the early stage of Ge adsorption on the SiC surface.

The atomic structure of substitutional adsorption of Ge on SiC(0001) was investigated by Diani et al. [10]. Based upon X-ray photoelectron spectroscopy (XPS) results, they verified Ge adatoms occupying the topmost Si sites of the Si-rich SiC(0001)-(3×3) surface, which is in agreement with the surfactant property of Ge. However, they also find a partial segregation of Ge toward SiC bulk region. Mansour et al. [11,12] performed a detailed experimental investigation of Ge adsorption on the (3×3) and $(\sqrt{3}\times\sqrt{3})R30^{\circ}$ reconstructed SiC(0001) surfaces. They verified that an annealing process at 400 °C, of the SiC surface covered with 1 monolayer (ML) of Ge, gives rise to Ge-tetramers with (4×4) surface periodicity. Increasing the annealing temperature, within a temperature window between 500 and 800 °C, the (4×4) structure disappears and the formation of 3D islands becomes evident. Further investigation find out that those islands are formed by Si atoms originated from the Si → Ge atomic exchange process.

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0039-6028/$ - see front matter © 2006 Elsevier B.V. All rights reserved.
doi:10.1016/j.susc.2005.12.045

Comparing the Ge adsorption processes, on the (3×3) and $(\sqrt{3} \times \sqrt{3})R30^\circ$ surfaces, they verified that the formation of Si islands is more evident on the (3×3) surface phase. Meanwhile, the formation of Ge wetting layer is more effective on the $(\sqrt{3} \times \sqrt{3})R30^\circ$ surface [11]. Based upon those experimental findings, we believe that an atomistic modeling is essential to improve our insight related to Ge covered SiC surfaces.

In this work we performed an ab initio total energy study of initial stage of Ge adsorption process on the $(\sqrt{3} \times \sqrt{3})R30^\circ$ and (3×3) SiC(0001) surfaces. We have examined a large number Ge adsorbed structural models. The energetic stability of the Ge adsorbed SiC(0001) surfaces was determined as a function of the Si and Ge concentrations. For the energetically more stable configurations we detailed the surface equilibrium geometries. In addition, we have performed a (exhaustive) comparative basis set analysis to describe the total energies and equilibrium geometries of the Si-terminated and Ge-adsorbed SiC(0001) surfaces.

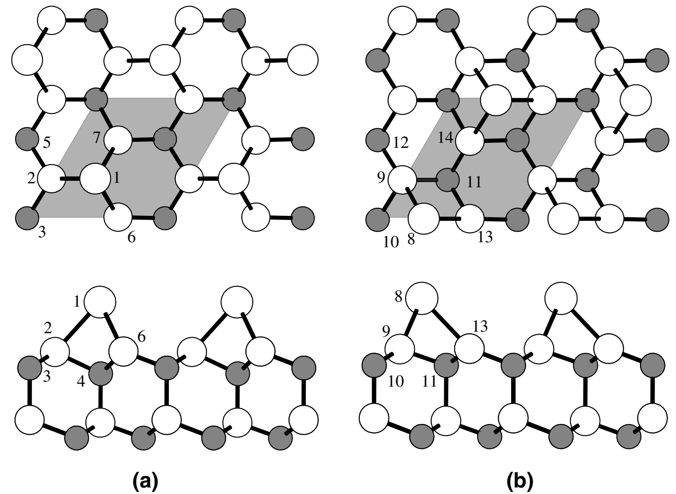

Fig. 1. Schematic representation of the SiC(0001)-$(\sqrt{3} \times \sqrt{3})R30^\circ$ surface. In (a) the topmost adatom lies on the T_4 site, and in (b) the topmost adatom lies on the H_3 site. The open circles represent the Si or Ge atoms, and the C atoms are represented by filled circles. The $(\sqrt{3} \times \sqrt{3})R30^\circ$ surface unit cells are indicated by the shaded areas.

2. Theoretical approach

The calculations were performed within the density functional theory, within the local density approximation. The electron–ion interaction was described by using norm-conserving fully separable pseudopotentials. The Kohn–Sham wave functions were expanded using linear combination of pseudoatomic orbitals [13]. We have used the following basis sets: (i) less accurate however (computationally) more efficient double-zeta (DZ), and (ii) well converged and very accurate double-zeta with polarization functions (DZP) [14]. The calculations were performed by using SIESTA code [15]. Two special **k** points and energy cutoff of 200 Ry, for the grid integration, were utilized to calculated the charge density. The SiC(0001) surfaces were simulated by using the slab method, with four bilayer of SiC plus a vacuum region of 10 Å. The dangling bonds of the bottom layer were saturated with hydrogen atoms. Equilibrium atomic positions were determined by relaxation within a force convergence criteria of 50 meV/Å.

3. Results and comments

Initially we examined the energetic stability and the equilibrium geometry of the Si-covered $(\sqrt{3} \times \sqrt{3})R30^\circ$ reconstructed 6H–SiC(0001) surface. Comparing the adsorption energies of Si adatoms lying on the T_4 (Si_{T_4}) and H_3 (Si_{H_3}) sites, sites 1 and 8 indicated in Fig. 1(a) and (b), respectively, we find that the Si_{T_4} configuration is energetically more favorable by 0.44 eV using the DZ basis set. Using a more accurate basis set, DZP, the Si_{T_4} configuration is energetically more stable by 0.52 eV. Those results are in accordance with previous (plane-wave) ab initio calculations, where the Si_{T_4} configuration is energetically more favorable, compared with the Si_{H_3} model, by 0.54 eV [16] and 0.60 eV [17] per $\sqrt{3} \times \sqrt{3}$ surface unit cell. The equilibrium geometry for the Si_{T_4} structure is summarized in Table 1. Again we find a good agreement between our calculated results (for both basis sets) and those obtained in Refs. [16–19]. Thus, we can infer that the DZ basis set describe very well the energetic and structural properties of Si-covered SiC(0001) surfaces.

So far we have verified the adequacy of our calculation procedure for the Si-covered SiC(0001)-$(\sqrt{3} \times \sqrt{3})R30^\circ$ surface, we next investigate the Ge adsorption process. For a Ge coverage of 1/3 ML, we considered six structural models on the $(\sqrt{3} \times \sqrt{3})R30^\circ$ surface (Fig. 1). For Ge adatoms lying on the topmost T_4 sites, Fig. 1(a), we have the Ge_{T_4} model, whereas for Ge adatoms on the H_3 sites, we have the Ge_{H_3} model [Fig. 1(b)]. For Ge adatoms occupying the Si sites of the first sublayer, site 2 (9), and the topmost Si adatom lying on the T_4 (H_3) site, we have the $Ge_{S_2(T_4)}$ ($Ge_{S_9(H_3)}$) model. Finally, for Ge adatoms siting on the C sites, site 4 (11), and keeping the topmost Si adatom lying on T_4 (H_3) we have the $Ge_{S_4(T_4)}$ ($Ge_{S_{11}(H_3)}$) model [3].

In order to infer the energetic stability of the Ge adsorbed $(\sqrt{3} \times \sqrt{3})R30^\circ$ surface, we compared the surface

Table 1
Equilibrium geometry for the Si_{T_4} and Ge_{T_4} structures

Structure	$z(1–2)$	$z(1–3)$	$z(1–4)$	$d(1–2)$	$d(2–4)$
Si_{T_4}, DZ	1.82	2.42	2.66	2.50	1.91
Si_{T_4}, DZP	1.78	2.33	2.58	2.46	1.88
Ab initio calculations [16]	1.75	–	–	2.42	–
Ab initio calculations [17]	1.71	2.25	2.50	2.41	1.88
X-ray diffraction [18]	1.61	–	2.40	2.31	1.84
Electron diffraction [19]	1.68	2.31	2.55	2.35	–
Ge_{T_4}, DZ	1.88	2.48	2.70	2.53	1.91
Ge_{T_4}, DZP	1.86	2.41	2.64	2.52	1.88

The vertical distance $[z(i-j)]$ and bond length $[d(i-j)]$ are in Å. The atomic labels are indicated in Fig. 1.

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