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First principles total energy calculations of the surface atomic structure of yttrium disilicide on Si(1 1 1)

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Abstract

We perform first principles total energy calculations to investigate the adsorption of yttrium silicide on Si. Our studies apply the density functional theory, and use the exchange and correlation potential energies according to the generalized gradient approximation within the Perdew, Burke, Ernzerhof parametrization. We study the formation of a two-dimensional (2D) structure of YSi_2 and the arrangement of a few layers of $YSi_{1.7}$ on Si(1 1 1). One monolayer of YSi_2 on Si(1 1 1) assembles in a 2D phase with (1×1) periodicity, which is composed of a layer of yttrium atoms on T_4 sites and a silicon bilayer on top. Similar to the structure of rare earth and $ScSi_2$ structures on Si(1 1 1), this bilayer of Si atoms resembles the ideal Si(1 1 1)–(1×1) surface, but rotated 180° with respect to the rest of the crystal. Additional layers of yttrium silicide on Si(1 1 1) build a hexagonal geometry similar to bulk YSi_2: graphite-like Si planes (with vacancies) intercalated with Y planes, and yielding a $(\sqrt{3} \times \sqrt{3})$ periodicity with a $YSi_{1.7}$ stoichiometry. As in the formation of a single layer of YSi_2, the surface is terminated by a Si bilayer similar to those of bulk Si along the (1 1 1) direction, but rotated 180°.

Keywords: Yttrium disilicide; Silicon surface; Atomic structure; First principles calculations

1. Introduction

Even though surface atomic structures of fundamental semiconductors, such as silicon and germanium, have been extensively investigated [1], there is still a great interest in the study of these surfaces when other materials are deposited on them. In particular, the adsorption of rare earth (RE) silicides on Si(1 1 1) surfaces has attracted the attention of researchers because these systems have technological applications [2–25]. The interfaces of RE silicides with Si(1 1 1) have very small lattice mismatches [2], sharp interfaces, and low Schottky barrier heights [3], making them ideal in devices, such as infrared detectors and rectifying contacts. Similar properties can be seen in the adsorption of silicides of transition metals such as YSi [4] and ScSi.

In this paper, we shall address studies of the growth of a few layers of YSi on the Si(1 1 1) surface. It has been reported that the adsorption of less than one monolayer of YSi on Si(1 1 1), reconstructs in a $(2\sqrt{3} \times 2\sqrt{3})R30^0$ [15,16] or (5×2) periodicities. For YSi coverage of one monolayer the adsorption takes place with a two-dimensional metallic structure, in a $p(1 \times 1)$ periodicity. At higher YSi coverage the reconstruction is of $(\sqrt{3} \times \sqrt{3})R30^0$ periodicity and a three-dimensional metallic silicide is obtained. Very recently a detailed surface structural study of the three-dimensional yttrium silicide epitaxially grown on Si(1 1 1) was done [25] using dynamical low energy electron diffraction (LEED). Accurate values were found of the atomic positions in the last surface planes. To our knowledge no theoretical calculations on this system has been performed and a first principles study of such system is desirable to compare with these new experimental data, and see if the calculations can correctly predict the right surface structure.

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We report first principles total energy calculations, to investigate the atomic structure of: (1) the two-dimensional (2D) formation of YSi_2 on Si(1 1 1) and (2) the deposition of a few layers of $YSi_{1.7}$ on Si(1 1 1). (1) For the 2D formation of YSi_2 we have considered two possible configurations: (a) in one model Si atoms of the silicide form bonds with Si atoms of the surface, and (b) in another model Y atoms form bonds with Si at the surface (see Fig. 1). Although there is a previous theoretical work in the same system, the authors have assumed the so-called BT_4 atomic geometry and optimized it [23]. (2) The growth of a few layers of $YSi_{1.7}$ on Si(1 1 1) was studied considering models [14–17], which have been initially proposed to explain the adsorption of RE elements on Si(1 1 1), but up to now, there are no theoretical calculations for YSi_2 on Si(1 1 1). These models consist of bulk-like Si bilayers without vacancies in the topmost plane. At the surface, nine atoms form the unit cell, three of RE elements and six of Si. However, there exist different possibilities of vacancies in the inner planes, where eight atoms per unit cell are considered, three of RE elements and five of Si.

(1) The vacancies in the top most Si graphitic layer can be either below the Si_{up} or the Si_{down} atoms as shown in Fig. 2.
(2) The stacking of the vacancies in the graphite-like planes can be either: one on top of the other, or two consecutive planes can be rotated by 60°, and 120° as shown in Fig. 3.

Our studies are carried out using the DFT formalism. We treat the exchange and correlation energies within the generalized gradient approximation (GGA) according to the Perdew, Burke, and Enzerholf (PBE) parameterization [27]. The paper is organized as follows: Section 2 describes the method, Section 3 is dedicated to the description of the results and discussion, and Section 4 is for the conclusions.

2. Computational technique

We perform first principles total energy calculations to study the atomic configuration of the adsorption of YSi_2

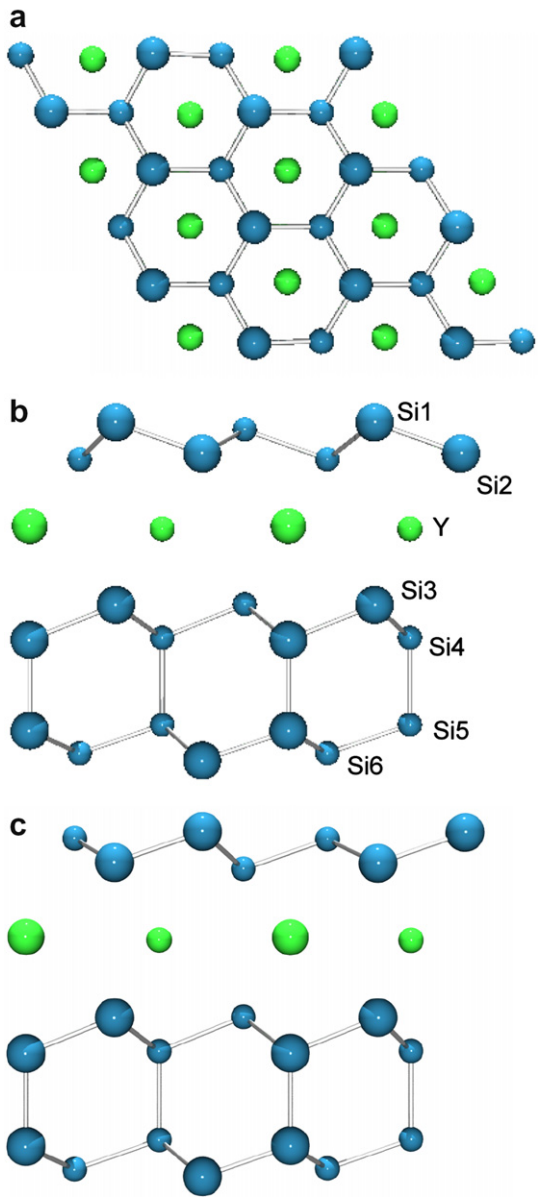

Fig. 1. Schematic representation of the Si(1 1 1)–(1 × 1) YSi_2 system (a) top view (b) side view. (c) The same as in (b), but the top Si bilayer is not rotated.

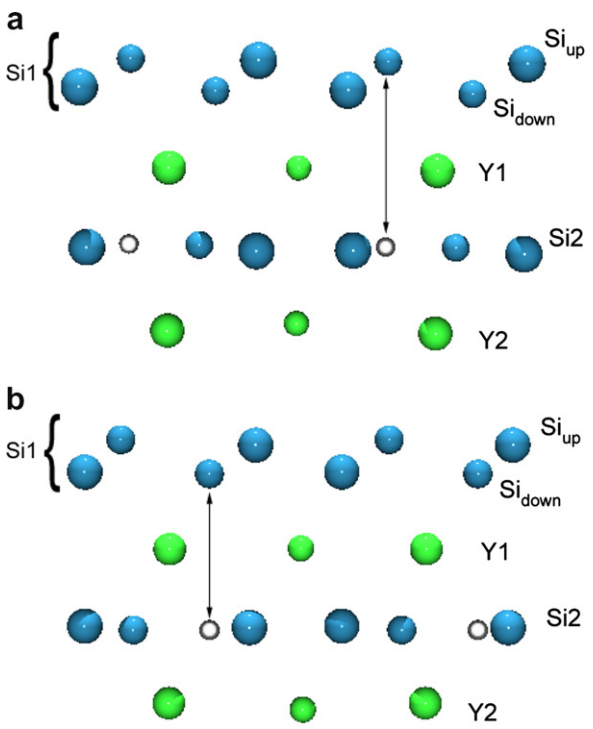

Fig. 2. (a) Surface model proposed by Roge et al. in which the vacancies are located below the Si_{up} atoms, and (b) surface model proposed by Martin-Gago et al. in which the vacancies are below the Si_{down} atoms.