Thin Solid Films 519 (2011) 5467–5472

Contents lists available at ScienceDirect

Thin Solid Films

journal homepage: www.elsevier.com/locate/tsf

Theoretical investigation of atomic structure and electronic properties of Ca/Si(110)-(2×1) reconstruction

A.Z. AlZahrani

Physics Department, Faculty of Science, King Abdulaziz University, P.O. Box 80203, Jeddah 21589, Saudi Arabia

ARTICLE INFO

Article history:
Received 28 September 2010
Received in revised form 1 March 2011
Accepted 2 March 2011
Available online 14 March 2011

Keywords:
Si(110) surface
Alkaline-earth metals
Ca adsorption
Density functional theory
Local density approximation
Ionic bonds
Surface states
Charge density

ABSTRACT

We have presented first-principles total-energy calculations for the adsorption of Ca metals onto a Si(110) surface. The density functional method was employed within its local density approximation to study the atomic and electronic properties of the Ca/Si(110) structure. We considered the (1×1) and (2×1) structural models for Ca coverages of 0.5 monolayer (ML) and 0.25 ML, respectively. Our total-energy calculations indicate that the (1×1) phase is not expected to occur. It was found that Ca adatoms are adsorbed on top of the surface and form a bridge with the uppermost Si atoms. The Ca/Si(110)-(2×1) produces a semiconducting surface band structure with a direct band gap that is slightly smaller than that of the clean surface. One filled and two empty surface states were observed in the gap; these empty surface states originate from the uppermost Si dangling bond states and the Ca 4 *s* states. It is found that the Ca–Si bonds have an ionic nature and complete charge being transferred from Ca to the surface Si atoms. Finally, the key structural parameters of the equilibrium geometry are detailed and compared with the available results for metal-adsorbed Si(110) surface, Ca/Si(001), and Ca/Si(111) structures.

1. Introduction

The adsorption of metal atoms on semiconductor surfaces has been the subject of an enormous number of experimental and theoretical investigations due to its possible technological and industrial applications. Recently, there have been many experimental works devoted to fabricating nanoscale electronic devices using self-assembled one-dimensional (1D) overlayer structures based on metallic adsorption onto semiconductor surfaces. These 1D structures have received immense interest due to the possibility of observing various exotic physical phenomena, such as formations of non-Fermi-liquid-like ground states, Peierls-like phase transitions, and order–disorder transitions, as well as the potential applications of these phenomena in nanotechnology [1–6]. Among the vast number of semiconductor materials, group-IV semiconductor surfaces (namely Si surfaces) are the keystones of most electronic devices and, hence, have been used in many different investigations. Despite that Si(001) and Si(111) surfaces have been intensively investigated upon different metallic adsorbates, there has been very little attention paid to the study of the adsorption of metallic atoms on the Si(110) surface. It is believed that the experimental difficulties in preparing a clean Si(110) surface could be considered as the main reason of such reluctance [7]. The difficulties in producing Si(110) have led Si(001) to be the most desired surface for microelectronics applications such as metal oxide semiconductor field effect transistors (MOSFETs). However, the Si(110) surface has recently been reinvestigated in an attempt to extend current fabrication technologies, not only because the existing MOSFET fabrication techniques are reaching fundamental physical limits, but also because the fabrication challenges for Si(110) including substrate planarization [8] and the growth of high-quality gate oxide layers [9] have been experimentally overcome. These technical developments suggest that Si(110) could be of great importance as a an accessible surface for electronics applications and be of significant potential in manufacture of semiconductor devices. Therefore, the emphasis is now on the need for further investigations of industrially important processes such as metal deposition on the Si(110) surface. To date, the atomic structure of the (110) surface of Si has been the subject of some controversy. Despite many works that suggest various reconstructions for clean Si(110) surface including the (1×1), (2×1), (5×1), (7×1), (9×1), (4×5), (5×4), (16×2), and (32×2) phases, it has been reported that only a (16×2) reconstruction can exist in a pure form and that all other various reconstructions must be temperature and dopant stabilized. However, this controversy suggests that there is no firm structural model for clean surface and/or metal-induced surface [10–20]. Using *ab initio* calculations, Stekolnikov et al. [21] have investigated different reconstructions of clean Si and Ge(110) surfaces using (1×1), (1×2), (2×1), c(2×2), (2×2),(3×1), (3×2), or (6×2) translational symmetry. It was found that the adatom-tetramer-interstitial (3×2) model stabilizes the Si and Ge surfaces, leading the Si(110) surface to

E-mail address: azalzahrani@kau.edu.sa.

0040-6090/$ – see front matter © 2011 Elsevier B.V. All rights reserved.
doi:10.1016/j.tsf.2011.03.009