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Ab initio calculations of surface structure and electronic properties caused by adsorption of Ca atoms on a Si(1 1 0) surface

A.Z. Alzahrani

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

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ABSTRACT

The adsorption of Ca metals onto a Si(1 1 0) surface has been theoretically investigated by first-principle total-energy calculations. We employed a local density approximation of the density functional theory as well as a pseudopotential theory to study the atomic and electronic properties of the Ca/Si(1 1 0) structure. The (1×1) and (2×1) surface structures were considered for Ca coverages of 0.5 and 0.25 ML, respectively. It is found that the (1×1) phase is not expected to occur even for rich Ca regime. It was found that Ca adatoms are adsorbed on top of the surface and form a bridge with the uppermost Si atoms. The most stable structure of Ca/Si(1 1 0)–(2×1) surface produces a semiconducting surface band structure with a direct band gap that is slightly smaller than that of the clean surface. We have observed one filled and two empty surface states in the gap region. These empty surface states originated from the uppermost Si dangling bond states and the Ca 4*s* states. Furthermore, the Ca–Si bonds have an ionic nature with almost complete charge transfer from Ca to the surface Si atoms. The structural parameters of the ground state atomic configuration are detailed and compared with the available results of metal-adsorbed Si(1 1 0) surface, Ca/Si(0 0 1), and Ca/Si(1 1 1) structures.

1. Introduction

Metallic adsorption on semiconductor surfaces has been the subject of an enormous number of experimental and theoretical investigations due to its possible technological and industrial applications. Based on metallic adsorption onto semiconductor surfaces there have been many experimental works devoted to fabricate nanoscale electronic devices using self-assembled one-dimensional (1D) overlayer structures. These 1D structures have received immense interest due to the possibility of various exotic physical phenomena such as formation 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 of the electronic devices and hence have been used in many different investigations. Apart from the most studied Si(1 0 0) and Si(1 1 1) surfaces for metallic adsorbates, there has been very little attention paid to the study of the adsorption of metallic atoms on the Si(1 1 0) surface. The main reason for this can be attributed to the experimental difficulties in preparing a clean Si(1 1 0) surface [7]. The difficulties in producing Si(1 1 0) have led Si(1 0 0) to be the most desired surface for microelectronics applications such as metal oxide semiconductor field effect transistors (MOSFETs). However, the Si(1 1 0) 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(1 1 0) including substrate planarization [8] and the growth of high-quality gate oxide layers [9] have been experimentally overcome. These technical developments suggest that Si(1 1 0) could be of great importance as a newly accessible surface for electronic applications. Therefore, the emphasis is now on the need for further investigations of industrially important processes such as metal deposition on the Si(1 1 0) surface. To date, the atomic structure of the (1 1 0) surface of Si has been the subject of some controversy. Despite many works that suggest various reconstructions for clean Si(1 1 0) 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 the 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]. Recently, Sakamoto et al. [21] have investigated the electronic structure of a single domain Si(1 1 0)–(16×2) surface using high-resolution angle-resolved photoelectron spectroscopy (ARPES) and scanning tunneling microscopy (STM)

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

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