Available online at www.sciencedirect.com
SCIENCE DIRECT®
Surface Science 585 (2005) 53–58
SURFACE SCIENCE
www.elsevier.com/locate/susc

Sb adsorption and desorption pathways on (2×1) and $c(4\times4)$ reconstructed Si(001) surfaces

Vinod Kumar Paliwal [1], Mahesh Kumar, S.M. Shivaprasad *

Surface Physics and Nanostructures Group, National Physical Laboratory, Dr. K.S. Krishnan Road, New Delhi 110 012, India

Received 22 September 2004; accepted for publication 8 April 2005
Available online 26 April 2005

Abstract

The role of initial surface reconstruction on the kinetics of heteroepitaxial growth of Sb on Si(001) surface is elucidated. The adsorption and desorption of Sb, from the clean-(2×1) and $c(4\times4)$ reconstructions of Si(001) surface, is investigated by in situ auger electron spectroscopy (AES) and low energy electron diffraction (LEED). Sb is adsorbed at room-temperature (RT) onto clean-(2×1) and $c(4\times4)$ reconstructed Si(001) surfaces at a base pressure of 3×10^{-11} Torr. At the very low flux rates adopted (0.06 monolayer/min), Sb grows epitaxially at RT and forms a (1×1) surface phase for coverages greater than 1.0 monolayer (ML) on both the (2×1) and $c(4\times4)$ surfaces. Residual thermal desorption studies done on these RT-adsorbed systems are observed to adopt different pathways. The '(2×1) case' results in an intermediate novel 0.6-ML (8×4) phase, while the '$c(4\times4)$ case' directly yields the 0.25-ML $c(4\times4)$ phase. The 0.25-ML Sb covered $c(4\times4)$ obtained from the Si(001)-$c(4\times4)$ phase is observed to be sharper than that obtained from the (2×1) reconstructed surface. Upon complete Sb desorption both the cases result in the clean Si(001)-(2×1) surface. The difference in desorption pathways is related to the Sb monolayer formation.

Keywords: Silicon; Antimony; Metal–semiconductor interfaces; Adsorption kinetics; Epitaxy; Low energy electron diffraction (LEED); Auger electron spectroscopy

1. Introduction

Applications of heteroepitaxial structures in nanoscale technology substantially tighten the demands on stability, and structural and compositional integrity [1,2]. Thus, tailoring desired interface properties by kinetic control is very important

* Corresponding author. Tel.: +91 11 25746270; fax: +91 11 25726938.
E-mail addresses: vkpaliwal@mail.nplindia.ernet.in (V.K. Paliwal), prasad@mail.nplindia.ernet.in (S.M. Shivaprasad).
[1] Present address: Department of Physics, Dyal Singh College, University of Delhi, Lodhi Road, New Delhi 110 003, India.

0039-6028/$ - see front matter © 2005 Elsevier B.V. All rights reserved.
doi:10.1016/j.susc.2005.04.013

for the fabrication of devices that exploit the exotic properties at nanodimensions. The ability to control the growth modes and resulting surface phases, by precise kinetic handles and desorption dynamics, can enable the formation of two-dimensional arrays of various phases with tunable properties. However, this atomic scale control encounters challenges due to growth kinetics that is strongly influenced by the rate limiting steps such as surface orientation, reconstruction, lattice-mismatch, interface stress, etc. along with the deposition rate and substrate temperature [2–4]. This has driven several very careful in situ studies towards the determination of the phase diagram of group-III and group-V metals on Si and GaAs surfaces to find recipes for obtaining pre-determined superstructural phases. Especially, the Sb/Si interface has great potential in forming δ-doped structures and surfactant-mediated Ge/Si heteroepitaxy and thus motivates such studies [5,6].

Among other parameters, surface reconstruction plays a crucial rate-limiting step in determining the structure and morphology of the nanostructures formed, consequently influencing their nanoscale electronic properties. We have recently reported the observation of new phases, viz ($5\sqrt{3}\times 5\sqrt{3}$-$R30°$) at 0.2 monolayer (ML) and (5×5) at 0.4 ML in the Sb/Si(1 1 1)-(7×7) system [7,8]. It is also shown that different adsorption and desorption pathways can result in entirely different geometric arrangements for the same adsorbate coverages [8]. Sb adsorption on Si(1 1 1) surface is extensively studied, as compared to that on Si(0 0 1)-(2×1) surface. The Sb/Si(0 0 1)-(2×1) interface has been probed by a variety of techniques [9–14], and theoretical calculations [15,16]. It is generally observed that for high temperature adsorption on the Si(0 0 1)-(2×1) surface Sb adatoms themselves form dimer rows perpendicular to the original Si dimer rows while relaxing the substrate reconstruction [10]. Limited, but controversial studies exist for substrate temperatures less than 550 °C, where the structure is observed to range from three-dimensional clusters, disordered layers to Sb–Sb dimers [6,9,11]. This disagreement in results can be due to differences in the formation conditions, as apparent from our previous studies on the Si(1 1 1)-(7×7) surface [7].

In this work, we have studied Sb adsorption/desorption for clean Si(0 0 1)-(2×1) surface. This is also the first report, on the study of Sb adsorption/desorption for the c(4×4) reconstructed Si(0 0 1) surface, to the best of our knowledge. The difference in the basic structure of the two reconstructions provides different adsorption sites for the adsorbate atoms and thus has prompted us to undertake a careful investigation of the adsorption/desorption processes in these systems. We have performed Sb adsorption at a low deposition rate of 0.06 ML/min. Residual thermal desorption studies, performed on the two systems, showed differences in the desorption sequence.

2. Experimental

The experiments are performed in an ultra-high vacuum chamber (Varian VT-112) operating at a base pressure of 3×10^{-11} Torr. The chamber is equipped with a single pass cylindrical mirror analyzer (CMA), which is used for auger electron spectroscopy (AES). An in situ four-grid optics with a concentric electron gun is used to observe the low energy electron diffraction (LEED) pattern. The sample is a 15×7 mm^2 rectangular piece cut from a commercially available p-type (Boron doping of 1×10^{15} atoms/cm^3) Si(0 0 1) wafer. Before introducing into the ultra-high vacuum chamber, the sample is cleaned by the modified Shiraki process [17] to remove the hydrocarbon contaminants and to form a clean SiO_2 epilayer. The sample is mounted between two Tantalum clips through which it is resistively heated to desired temperatures. The sample temperature is measured by a thermocouple (W–Re5%/W–Re25%) mounted behind the sample and an optical pyrometer. The sample is thoroughly degassed at 600 °C and flashed to 1200 °C when the contaminant signals in AES are reduced to undetectable levels and the LEED showed a sharp, double-domain (2×1) pattern. Si-c(4×4) surface without any detectable carbon impurity was prepared, using a procedure similar to Wang et al. [18], by cooling the sample from about 1100 °C, keeping it at 650 °C for about 5 min and then cooling down to RT in 5 min. Antimony (Sb) is adsorbed from a home-made Tanta-