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ScienceDirect
Surface Science 601 (2007) 837–843
SURFACE SCIENCE
www.elsevier.com/locate/susc

Atomic geometry and electronic properties of the Ge(1 1 1)2 × 1-Sb surface studied by scanning tunneling microscopy/spectroscopy and core-level photoemission

M. Kuzmin *, P. Laukkanen, R.E. Perälä, M. Ahola-Tuomi, I.J. Väyrynen

Department of Physics, University of Turku, FIN-20014 Turku, Finland

Received 8 September 2006
Available online 11 December 2006

Abstract

By scanning tunneling microscopy and spectroscopy (STM/S) and high-resolution core-level photoemission using synchrotron radiation, we have investigated the atomic structure and electronic properties of Sb-induced 2 × 1 reconstruction on Ge(1 1 1). Our results support well the zigzag-chain model proposed for this phase in the literature; in particular, the STM images visualize the Sb zigzag (Seiwatz) chain in a real space, and the STS *I–V* spectrum suggests this surface to be semiconducting, in good agreement with the atomic configuration proposed. However, a closer inspection of the STM results does not support the buckling of Sb chains reported in earlier studies. Moreover, the analysis of the Sb 4d core-level line shape of the (2 × 1) reconstruction shows that the bonding state of the Sb atoms is very similar, suggesting an unbuckled Seiwatz chain. In addition, the Ge 3d core-level emission reveals only one component, giving evidence for the ideal bulk-terminated structure of the Ge substrate.

Keywords: Single crystal surfaces; Surface relaxation and reconstruction; Scanning tunneling microscopy and spectroscopy; Synchrotron radiation photoelectron spectroscopy; Germanium; Antimony

1. Introduction

Due to fundamental and technological interests, the behavior of group-*V* adsorbates on Si(1 1 1) and Ge(1 1 1) surfaces has been studied both experimentally and theoretically in the last two decades (e.g. see Refs. [1,2] and references therein). In particular, it has been shown that in such systems, a full passivation can be achieved through the elimination of the surface dangling bonds completely, and that several adsorbate-overlayer geometries can be observed depending on the covalent radius of the group-V atom. One example is the Sb/Ge(1 1 1) surface with the adsorbate coverage of one monolayer (ML) [3–7], of which structural and electronic properties are studied in this paper.

In early low-energy electron diffraction (LEED) studies, a (1 × 1) structure has been reported for the Sb/Ge(1 1 1) surface at 1 ML [3]. On the basis of LEED *I–V* curves, a model in which the Sb atoms substitute the first Ge layer on the bulk-terminated Ge(1 1 1) surface (i.e. the so-called substitutional (1 × 1) model) was proposed. Later on, a (2 × 1) structure has been observed for the 1-ML Sb/Ge(1 1 1) surface in Ref. [4]. Using X-ray diffraction [4], X-ray standing waves [5,6], surface extended X-ray absorption fine structure techniques [5], and core-level photoemission [5], it has been revealed that the (2 × 1) periodicity is due to the zigzag (Seiwatz) chains which the Sb atoms arrange on the bulk-truncated Ge(1 1 1) substrate (Fig. 1). In such a structure, the Sb atoms occupy the top side on the ideally bulk-terminated Ge(1 1 1). Furthermore, the

* Corresponding author.
E-mail address: m.kuzmin@mail.ioffe.ru (M. Kuzmin).

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doi:10.1016/j.susc.2006.11.029

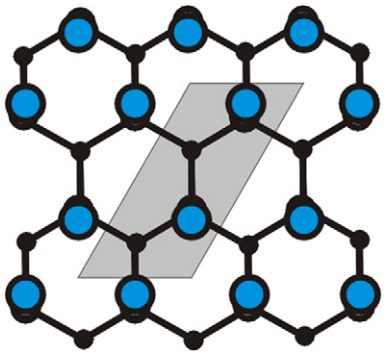

Fig. 1. Top view of the zigzag-chain structure of the Sb/Ge(1 1 1)-(2 × 1) reconstruction at 1 ML. The large circles represent the Sb atoms. The unit cell is shadowed.

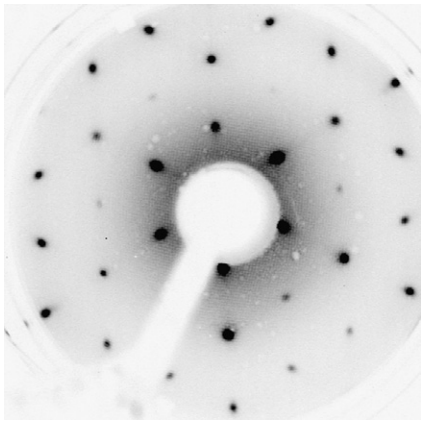

Fig. 2. A LEED pattern of the 1-ML (2 × 1)-Sb. The electron energy is 43 eV.

Sb–Ge bonds are slightly tilted, and the upper Ge layers exhibit a small relaxation [4,7]. This structure, however, has not been examined by direct experimental techniques, such as scanning tunneling microscopy (STM).

In this work, we visualize the chainlike structure of the 1-ML Sb/Ge(1 1 1)-(2 × 1) surface in a real space and show atomic-resolution STM images that confirm the zigzag-chain geometry of this reconstruction. We also present scanning tunneling spectroscopy (STS) data, which are well consistent with the above structural arrangement and indicate the (2 × 1) phase to be semiconducting. The STM line profiles, however, do not support the buckling along the zigzag chains, which was proposed in the previous investigations [4,7]. Moreover, the analysis of the Sb 4d core-level line shape, measured by high-resolution photoelectron spectroscopy with synchrotron radiation, reveals that the Sb 4d spectra include only one component, which also disagrees with the buckling. In addition, the Ge 3d emission can be also fitted by only one component, thus proposing the Ge(1 1 1) substrate to have an ideal bulk-terminated structure without noticeable surface relaxations of upper Ge layers.

2. Experimental

The measurements were performed in two separate ultra-high vacuum (UHV) systems. The STM/STS experiments were carried out in the UHV system with a base pressure of 5×10^{-11} mbar equipped with Omicron scanning probe microscope, LEED, and ion sputtering facilities. The STM images were acquired in the constant-current mode. The tunneling spectra were taken at every raster point of the topography image and averaged over a scanning area. The photoemission experiments were done on Beamline 33 at the MAX-lab synchrotron radiation facility in Lund, Sweden. The Ge 3d and Sb 4d core-level spectra were measured using an angle-resolved photoelectron spectrometer with an angle resolution of ~2°. The total energy resolution was better than 100 meV. The core-level binding energy (BE) was referred to the Fermi-level position of a metallic Ta sample in good electric contact with the Ge samples. All the measurements reported in this paper were conducted at room temperature (RT) under the pressure below 1×10^{-10} mbar.

The Ge samples were cut from an Sb-doped (n-type) (1 1 1) wafer. In the both UHV systems, the sample cleaning was carried out by repeated cycles of 1.0-keV Ar^+ sputtering at 400 °C and subsequent annealing at 620 °C until an excellent $c(2 \times 8)$ LEED pattern with sharp fractional-order spots and a low background was displayed. The sample heating was performed by direct current. Temperature was measured by an infrared pyrometer.

Sb was deposited from a W-filament evaporator. The deposition rate was measured by a quartz-crystal microbalance. 1 ML of adsorbate atoms was referred to as the atomic density on the bulk-truncated Ge(1 1 1) surface (7.22×10^{14} atoms/cm^2), which corresponds to the Sb-film thickness of 2.3 Å. About 1.5 ML of Sb was deposited onto the clean Ge(1 1 1)$c(2 \times 8)$ surface at RT, followed by annealing at 500 °C. This led to a replacement of the $c(2 \times 8)$ LEED spots of the clean substrate by the sharp (2 × 1) spots of the Sb/Ge(1 1 1) (Fig. 2), in agreement with previous observations [4]. As shown below, STM verified the (2 × 1) periodicity for this surface and showed the (2 × 1) phase to cover practically the whole surface area. These results also support the theoretical calculations in [7], according to which the (2 × 1) phase of the 1-ML Sb/Ge(1 1 1) is energetically more stable than the (1 × 1) geometry. Furthermore, the $(\sqrt{3} \times \sqrt{3})$ configuration with an Sb trimer centered on the T4 site was reported to be another favorable structure of the 1-ML Sb/Ge(1 1 1) [7]. In our experiment, however, no $\sqrt{3}$ phase was detected for the Sb/Ge(1 1 1), agreeing well with the previous experimental work [4–6].

3. Results and discussion

3.1. STM

A large-scale STM image of the Ge(1 1 1)2 × 1-Sb surface, taken at a sample bias voltage (V_S) of +2.9 V