

# High-resolution core-level photoemission study of Ge(1 1 1) $2 \times 1$ -Sb and Ge(1 1 1)( $\sqrt{3} \times \sqrt{3}$ ) $R30^\circ$ -Bi reconstructions

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## Abstract

Using high-resolution core-level photoelectron spectroscopy with synchrotron radiation, we have studied Ge(1 1 1) $2 \times 1$ -Sb and Ge(1 1 1)( $\sqrt{3} \times \sqrt{3}$ ) $R30^\circ$ -Bi reconstructions formed at the metal coverage of 1 and 1/3 monolayers, respectively. The spectral line shape analysis shows that for the both surfaces, the Ge 3d emission includes one component, giving evidence for the bulk-terminated structure of the Ge substrate in these phases. The Bi 5d emission from the Ge(1 1 1)( $\sqrt{3} \times \sqrt{3}$ ) $R30^\circ$ -Bi surface reveals an intense component related to the Bi atoms at the T4 site in the  $\sqrt{3}$  structure, in agreement with previous *ab initio* calculations. Another small Bi 5d component is assigned to Bi–Bi bondings in metallic Bi clusters. The Sb 4d spectra of the Ge(1 1 1) $2 \times 1$ -Sb surface can be reproduced well by a single component, suggesting that the Sb atoms in the Seiwatz chains have similar bonding configuration.

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## 1. Introduction

The behavior of group-V adsorbates, such as P, As, Sb, and Bi, on Si(1 1 1) and Ge(1 1 1) surfaces has been the subject of various experimental and theoretical investigations in the last two decades (e.g. see Refs. [1,2] and references therein). In particular, these studies are motivated by the possibility to use group-V metals as surfactants to improve the epitaxial growth of the strained Si/Ge heterojunctions [3,4]. Moreover, the group-V metals can also be utilized for the delta doping of elemental semiconductors [5].

From the fundamental viewpoint, the group-V metal-induced phases on Si(1 1 1) and Ge(1 1 1) represent an interesting example of the surface structures in which the surface dangling bonds are fully passivated and in which the substrate has a bulk-terminated atomic configuration [1,2]. In this case, the adsorbate overlayer geometry is expected to be controlled by the physical mechanisms that are driven by the strain relief. In fact, the adsorbate

structures of the group-V/Si(1 1 1) and /Ge(1 1 1) surfaces depend on the covalent radius of the group-V metal, and a full passivation of the dangling bonds can be achieved with different overlayer geometries. For example, the Bi/ and Sb/Ge(1 1 1) surfaces have very different surface unit cells [6–12]. A low-energy electron diffraction (LEED) study has shown that Bi induces a ( $\sqrt{3} \times \sqrt{3}$ ) $R30^\circ$  periodicity at the coverage of 1/3 monolayer (ML) [6]. On the basis of LEED *I*-*V* curves, it was found that in this structure, the Bi adatoms are located at the T4 site, as shown in Fig. 1(a), and that the first two layers of the Ge(1 1 1) substrate are significantly displaced from their ideal bulk positions [6]. These observations have been well supported by *ab initio* calculations according to which the T4 structure of the Ge(1 1 1)( $\sqrt{3} \times \sqrt{3}$ ) $R30^\circ$ -Bi in Fig. 1(a) is energetically stable at 1/3 ML [12]. At 1 ML, the milkstool structure (i.e. the  $\sqrt{3} \times \sqrt{3}$  trimer geometry) shown in Fig. 1(b) is favorable [12].

In contrast, Sb on Ge(1 1 1) forms a different structure [6–11]. At 1 ML, a substitutional (1  $\times$  1) adsorbate geometry was found in early LEED investigation [6], while later studies (Refs. [8–10]) have reported a (2  $\times$  1) configuration. Using X-ray diffraction [8], X-ray standing waves [9,10], surface extended X-ray absorption fine structure techniques [9], and core-level photoemission [9], it has been shown that in the Ge(1 1 1)(2  $\times$  1)-Sb reconstruction, the Sb atoms occupy

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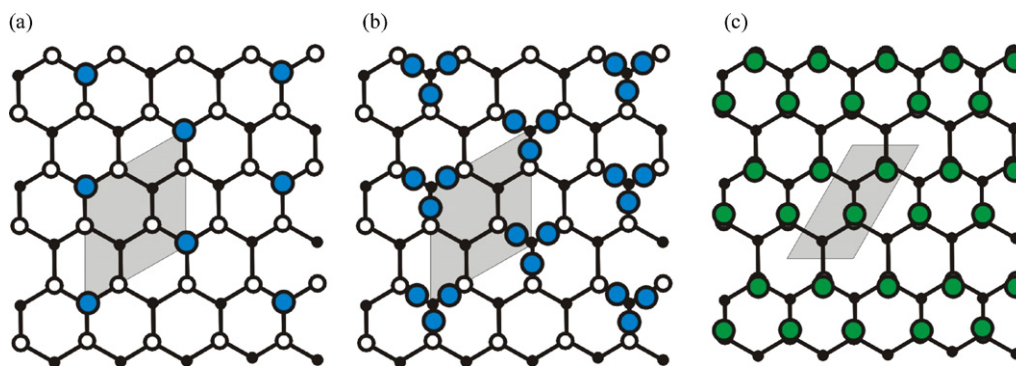


Fig. 1. Top view of the atomic models of the Bi/ and Sb/Ge(1 1 1) reconstructions. (a) T4  $\sqrt{3}$  structure of the Bi/Ge(1 1 1) surface at 1/3 ML. (b) The milkstool structure (i.e.  $\sqrt{3} \times \sqrt{3}$  trimer geometry) of the Bi/Ge(1 1 1) at 1 ML. (c) The  $(2 \times 1)$  zigzag chain structure of the Sb/Ge(1 1 1) at 1 ML. The large circles represent the group-V atoms. The unit cells are shadowed.

the top site and form zigzag (Seiwatz) chains on the almost bulk-truncated substrate which exhibits only small relaxations (Fig. 1(c)). Moreover, the Sb chains were proposed to have a small buckling [8]. These results have also been supported by the first-principle calculation in Ref. [11], where the  $2 \times 1$  is reported to be favorable for the Sb/Ge(1 1 1) at 1 ML.

The group-V/Ge(1 1 1) reconstructions, however, require a further examination by complementary experimental techniques in order to confirm the atomic structure of these systems and to elucidate a role of adsorbate atoms itself in the formation of the group-V metal-induced phases on Ge(1 1 1) and Si(1 1 1). In this work, we apply high-resolution core-level photoelectron spectroscopy using synchrotron radiation to investigate the Bi/ and Sb/Ge(1 1 1) surface phases formed at 1/3 and 1 ML, respectively. Previously, core-level photoemission has been utilized to examine the Ge(1 1 1) $2 \times 1$ -Sb surface [9]; however, in that study the overall resolution was only between 0.35 and 0.40 eV. Here we present the Ge 3d and Sb 4d core-level spectra for the Ge(1 1 1) $2 \times 1$ -Sb, taken with improved energy resolution, and also the Ge 3d and Bi 5d spectra for the Ge(1 1 1)( $\sqrt{3} \times \sqrt{3}$ ) $R30^\circ$ -Bi which, to our knowledge, has not been the subject of photoemission studies earlier. In this paper we discuss various aspects of the atomic and electronic structures of the both reconstructions in the context of the present results and the previous ones found in the literature.

## 2. Experimental

The experiments were carried out on Beamline 33 at the MAX-lab synchrotron radiation facility in Lund, Sweden. The core-level spectra were taken using an angle-resolved photoelectron spectrometer with an angular resolution of  $\sim 2^\circ$ . 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 spectra were acquired at room temperature (RT) under the residual pressure of  $4 \times 10^{-11}$  Torr.

The Ge samples were cut from an Sb-doped (n-type) (1 1 1) wafer. The sample cleaning was carried out by repeated cycles of 1.0-keV Ar<sup>+</sup> sputtering at 400 °C and subsequent annealing the sample at 620 °C until an excellent  $c(2 \times 8)$  LEED pattern

with sharp fractional-order spots and a low background was displayed. Fig. 2(a) shows a typical pattern obtained in this study. The sample heating was performed by direct current. Temperature was measured by an infrared pyrometer.

Bi and Sb were deposited from W-filament evaporators. The deposition rate was measured by a quartz-crystal microbalance. One monolayer (1 ML) of adsorbate atoms was referred to as the atomic density on the bulk-terminated Ge(1 1 1) surface ( $7.22 \times 10^{14}$  atoms/cm<sup>2</sup>), i.e. 1 ML = 2.5 Å for Bi and 2.3 Å for Sb. About 1.5 ML of Bi was deposited onto the clean Ge(1 1 1) $c(2 \times 8)$  at RT, followed by a post-deposition anneal at 320 °C. This resulted in a ( $\sqrt{3} \times \sqrt{3}$ ) $R30^\circ$  structure (Fig. 2(b)) with a Bi coverage of 1/3 ML (in short,  $\sqrt{3}$ -Bi) as in the previous study [6]. The 1-ML Sb/Ge(1 1 1)( $2 \times 1$ ) surface was prepared by deposition of about 1.5 ML Sb onto the Ge(1 1 1) $c(2 \times 8)$  at RT, followed by annealing at 500 °C. The LEED pattern is shown in Fig. 2(c). This observation is in good agreement with the experimental results in Refs. [8–10] and the theoretical calculation in [11] according to which the ( $2 \times 1$ ) structure of Sb/Ge(1 1 1) at 1 ML is more favorable than the ( $1 \times 1$ ) structure. In addition to the ( $2 \times 1$ ), a ( $\sqrt{3} \times \sqrt{3}$ ) configuration with one Sb trimer centered on the T4 site is another favorable structure of Sb/Ge(1 1 1) [11]. In our study, however, no sign of the  $\sqrt{3}$  periodicity was found in LEED, agreeing with the previous experimental observations [8–10]. Moreover, our very recent scanning-tunneling-microscopy (STM) experiment [13] verified (by a direct real-space method) that the Sb atoms arrange the ( $2 \times 1$ ) Seiwatz chains on Ge(1 1 1), and that the structure covers practically the whole surface area, whereas no  $\sqrt{3}$  phase was detected. Thus, we conclude that the procedure used in this study results in the well-ordered ( $2 \times 1$ )-Sb structure at 1 ML.

## 3. Results and discussion

### 3.1. Ge 3d

Fig. 3 shows Ge 3d spectra of the ( $2 \times 1$ )-Sb and  $\sqrt{3}$ -Bi surfaces, taken with the normal emission angle ( $\theta_e = 0^\circ$ ) at two different photon energies ( $h\nu = 70$  and 90 eV), together with their decomposition. The background was removed by the Shirley's

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