

# Electronic structure of the Sb-induced $\text{Si}(1\ 1\ 3)2 \times 5$ surface

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## Abstract

The surface electronic structure of  $\text{Sb}/\text{Si}(1\ 1\ 3)2 \times 5$  was investigated by angle-resolved photoemission spectroscopy experiments. This reveals  $\text{Sb}/\text{Si}(1\ 1\ 3)2 \times 5$  to have three surface bands with anisotropic two-dimensional characteristics. The band widths of the surface bands along  $[1\ \bar{1}\ 0]$  is larger than along  $[3\ 3\ \bar{2}]$ . The number of surface bands of  $\text{Sb}/\text{Si}(1\ 1\ 3)2 \times 5$  and their band dispersions along  $[1\ \bar{1}\ 0]$  and  $[3\ 3\ \bar{2}]$  are quite analogous with those of  $\text{Sb}/\text{Si}(1\ 1\ 3)2 \times 2$  composed of Sb adatom and Si tetramer chains. The electronic structure analogy suggests that  $\text{Sb}/\text{Si}(1\ 1\ 3)2 \times 5$  and  $\text{Sb}/\text{Si}(1\ 1\ 3)2 \times 2$  have common building blocks such as Sb adatom and Si tetramer chains. © 2006 Elsevier B.V. All rights reserved.

**Keywords:** Silicon; Antimony; Self-assembly; One-dimensional structure; Surface reconstruction; Photoemission spectroscopy

## 1. Introduction

Atomic wires have attracted much interest for studies related to exotic phenomena in one-dimensional (1D) electron systems such as Luttinger liquid [1], Peierls instability [2–4], 1D ferromagnetism [5], and a 1D Mott–Hubbard insulator [6]. This has encouraged the fabrications of various atomic wires on surfaces [1,2,5–8]. In general, an atomic wire on a surface is provided in the form of a two-dimensional (2D) array rather than a single atomic wire. A long-range order across atomic wires is related to an interwire (transverse) interaction between atomic wires so that atomic wires in the form of a 2D array are called quasi-1D ones rather than ideal 1D ones. The transverse interactions are due to various origins depending on physical properties of atomic wires: the transverse component of a nesting vector on a quasi-1D charge density wave [9] and a transverse spin–spin interaction on a quasi-1D Mott–Hubbard insulator [10].

One of transverse interactions is two competing periodicities [11], which results in a series of phases. A representative structure due to two competing periodicities is the Devil's staircase [11], as recently observed on  $\text{Pb}/\text{Si}(1\ 1\ 1)$  [12]. A competing interaction between  $\text{Pb}/\text{Si}(1\ 1\ 1)\sqrt{3} \times \sqrt{3}$  and  $\text{Pb}/\text{Si}(1\ 1\ 1)\sqrt{3} \times \sqrt{7}$  was suggested to produce various commensurate phases, where the 1D strips of  $\sqrt{3} \times \sqrt{3}$  and  $\sqrt{3} \times \sqrt{7}$  are arranged alternatively [12]. Besides,  $2 \times n$  phases ( $n$  is an integer) on  $\text{Si}(1\ 0\ 0)$  are provided by a competing interaction between the dimer chain of  $\text{Si}(1\ 0\ 0)2 \times 1$  and its dimer vacancy line [13], and  $1 \times n$  phases on  $\text{O}/\text{Ag}(1\ 1\ 0)$  are based on the two building blocks, Ag chains with and without oxygen [14]. Similarly, two competing periodicities were also reported on  $\text{H}/\text{Si}(1\ 1\ 3)$ , where  $2 \times n$  ( $n = 13, 7, 5,$  and  $2$ ) phases were found with increasing H coverage [15]. The sequential phase transitions were explained in terms of a competing interaction between the  $\text{H}/\text{Si}(1\ 1\ 3)2 \times 2$  structure and its domain wall, as observed using scanning tunneling microscopy (STM) [15].  $\text{Sb}/\text{Si}(1\ 1\ 3)$  also produces sequential phase transitions with increasing Sb coverage ( $\theta_{\text{Sb}}$ ):  $\text{Sb}/\text{Si}(1\ 1\ 3)1 \times n$  ( $1 \times n$ -Sb hereafter),  $\text{Sb}/\text{Si}(1\ 1\ 3)2 \times 5$  ( $2 \times 5$ -Sb hereafter), and

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Sb/Si(113) $2 \times 2$  ( $2 \times 2$ -Sb hereafter) [16]. This motivated us to investigate the electronic structure of  $2 \times 5$ -Sb in comparison with  $2 \times 2$ -Sb by angle-resolved photoemission spectroscopy (ARPES) experiments.

## 2. Experimental

The photoemission measurements were performed at the beamline BL-18A of photon factory, high energy accelerator research organization (KEK) [17]. The nominal energy and angle resolutions were better than 150 meV and  $1^\circ$ , respectively. Energy bands were measured using a photon energy of 11 eV. Clean Si(113) $3 \times 2$  was prepared by the repeated cycles of flashing at 1200 °C and subsequential annealing at 900 °C, as confirmed by low energy electron diffraction (LEED) patterns with clear non-integer spots. Sb atoms were deposited using quartz crucibles, and relative  $\theta_{\text{Sb}}$  was calibrated from the intensity ratio of Sb 3d and Si 2p spectra.

## 3. Results and discussion

The  $1 \times n$ -Sb,  $2 \times 5$ -Sb, and  $2 \times 2$ -Sb phases were sequentially observed with increasing  $\theta_{\text{Sb}}$  on clean Si(113) $3 \times 2$ , as reported previously [16,18], while similar phase transitions were also found on Cs/Si(113) [19] and H/Si(113) [15]. Fig. 1 shows the energy bands of  $2 \times 5$ -Sb along  $[1\bar{1}0]$ . The highly dispersive band B with a band width (BW) larger than 1.5 eV, not expected for a surface band on a semiconductor surface, is assigned as a bulk band [17]. Other three bands are located at bulk band gaps and, consequently, are assigned safely as surface bands, where the three surface bands, S1, S2, and S3, have binding energies (BE) of 0.6, 1.08, and 1.64 eV at  $\bar{\Gamma}$ , respectively. The three surface bands are dispersive along  $[1\bar{1}0]$ , while the S3 band has a larger BW of 0.64 eV than the S1 and S2 bands with BW's of 0.35 and 0.45 eV, respectively. In comparison, the dispersions along  $[3\bar{3}\bar{2}]$  of the three surface bands behave differently, as shown in Fig. 2. Along  $[3\bar{3}\bar{2}]$ , the S1, S2,

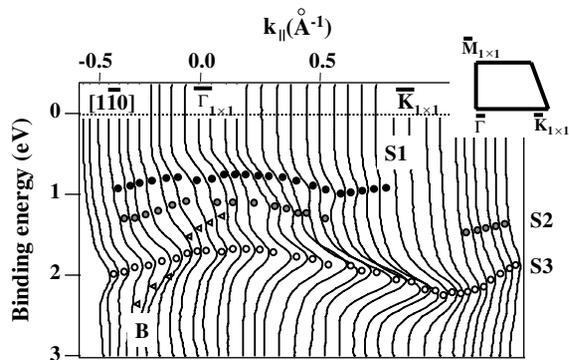


Fig. 1. Energy bands of Sb/Si(113) $2 \times 5$  shown in angle-resolved photoemission spectra along  $k_{\parallel}$  ( $[1\bar{1}0]$ ) using a photon energy of 11 eV, where the Brillouin zone of Si(113) $1 \times 1$  is drawn in the inset. The three surface bands, S1, S2, and S3, are denoted by different circles and the bulk band B is denoted by triangles.

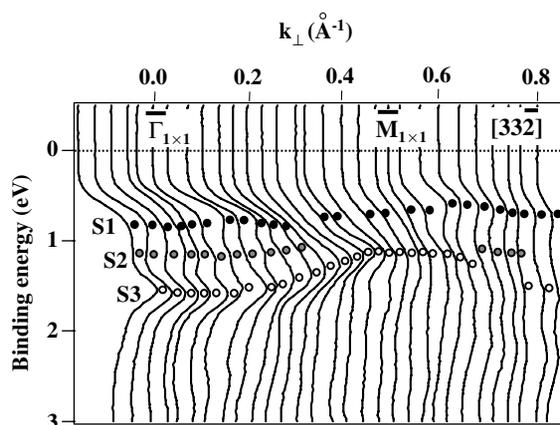


Fig. 2. Energy bands of Sb/Si(113) $2 \times 5$  shown in angle-resolved photoemission spectra along  $k_{\perp}$  ( $[3\bar{3}\bar{2}]$ ) using a photon energy of 11 eV. The three surface bands, S1, S2, and S3, are denoted by different circles.

and S3 bands have smaller BW's of 0.2, 0.15, and 0.52 eV, respectively, than along  $[1\bar{1}0]$ . The ratios ( $\text{BW}_{[1\bar{1}0]}/\text{BW}_{[3\bar{3}\bar{2}]}$ ) of BW's along  $[1\bar{1}0]$  and  $[3\bar{3}\bar{2}]$  are, thus, 1.8 (S1), 3.0 (S2), and 1.2 (S3). This indicates that the three surface bands have anisotropic 2D characteristics, while the S2 band is close to a quasi-1D one; electrons on  $2 \times 5$ -Sb are delocalized along  $[1\bar{1}0]$  and are relatively localized along  $[3\bar{3}\bar{2}]$ . The coexistence of surface bands with different dimensional characteristics on  $2 \times 5$ -Sb is similar with the energy bands of In atomic wires on In/Si(111) $4 \times 1$  with two quasi-1D bands and an ideal 1D band, where recent ARPES experiments suggested that only quasi-1D bands are related to interwire interactions between In atomic wires and contribute to a long-range order across In atomic wires [3].

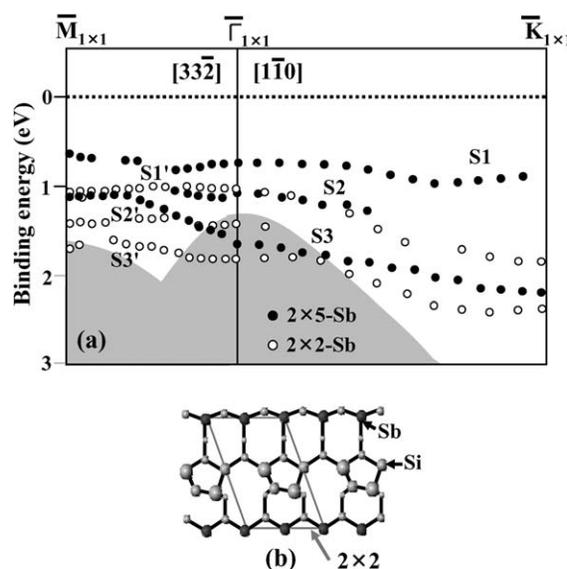


Fig. 3. (a) Energy bands of Sb/Si(113) $2 \times 5$  (solid circles) along  $[1\bar{1}0]$  and  $[3\bar{3}\bar{2}]$  are drawn in comparison with those of Sb/Si(113) $2 \times 2$  (open circles), where the shaded region is a bulk-projected band and the energy bands of Sb/Si(113) $2 \times 2$  are redrawn from An et al.'s report [18]. (b) Atomic structure of Müssig et al.'s adatom-tetramer model of Sb/Si(113) $2 \times 2$  [22].

The surface bands of  $2 \times 5$ -Sb along  $[1\bar{1}0]$  and  $[3\bar{3}2]$  are drawn in Fig. 3(a) in comparison with  $2 \times 2$ -Sb [18].  $2 \times 2$ -Sb also has three surface bands with different dimensional characteristics, where the three surface bands of  $2 \times 2$ -Sb, S1', S2', and S3', are denoted by open circles in Fig. 3(a) [18]. The atomic structure of  $2 \times 5$ -Sb is unknown up to now, but the comparison of the surface bands of  $2 \times 5$ -Sb with  $2 \times 2$ -Sb provides a clue for an atomic structure of  $2 \times 5$ -Sb. One may notice that the surface bands of  $2 \times 5$ -Sb are quite similar with those of  $2 \times 2$ -Sb except the overall binding energy shift by 0.2 eV. The electronic structure analogy may reflect that  $2 \times 5$ -Sb and  $2 \times 2$ -Sb have common building blocks. Nevertheless, we do not exclude that an atomic structure of  $2 \times 5$ -Sb, not sharing a common building block with  $2 \times 2$ -Sb, could explain the analogy of the surface bands.

Firstly, we consider an atomic structure of  $2 \times 5$ -Sb which is not related to one of  $2 \times 2$ -Sb. One of possible atomic structures is based on the bulk-terminated Si(113) $1 \times 1$  structure. It was suggested that Sb atoms of Sb/Si(111) $1 \times 1$  are located at the three-fold sites of the bulk-terminated Si(113) $1 \times 1$  structure saturating all Si dangling bonds [20]. Similarly, an atomic structure of  $2 \times 5$ -Sb can be built, where Sb atoms, located at the three-fold sites, should be arranged to satisfy the long-range order of  $2 \times 5$ . Two representative arrangements of Sb atoms producing the long-range order of  $2 \times 5$  are

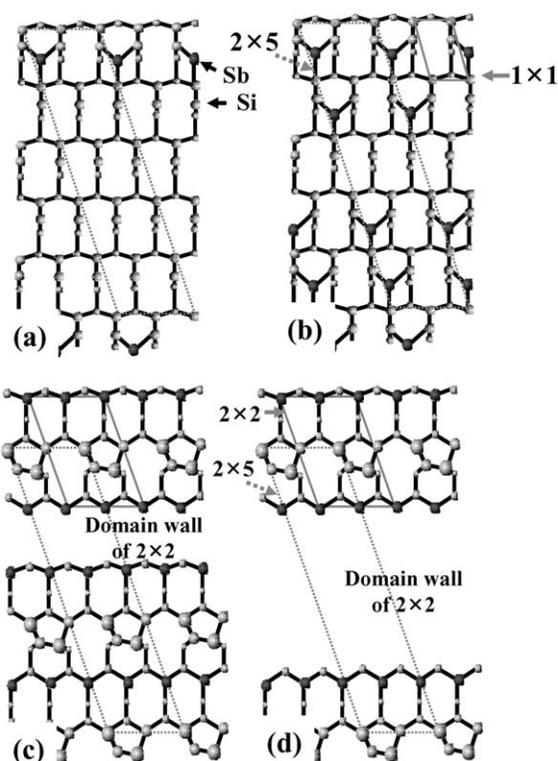


Fig. 4. Tentative atomic structure models of Sb/Si(113) $2 \times 5$ . The atomic structure models in (a)–(b) and (c)–(d) are based on the bulk-terminated Si(113) $1 \times 1$  structure and Müssig et al.'s adatom–tetramer model of Sb/Si(113) $2 \times 2$  [22], respectively.

shown in Fig. 4(a) and (b). The hybridized Sb–Si and unsaturated Si dangling bonds of the structures are expected to produce surface bands with different BW ratios ( $BW_{[1\bar{1}0]}/BW_{[3\bar{3}2]}$ ), though it is not obvious to assign the three surface bands of  $2 \times 5$ -Sb to the hybridized Sb–Si and unsaturated Si dangling bonds.

Secondly, we adopt the fact that the analogy of the surface bands of  $2 \times 5$ -Sb with  $2 \times 2$ -Sb indicates the existence of common building blocks between them. Here, we need to introduce the atomic structure of  $2 \times 2$ -Sb. Since most adsorbates,  $H_2$  molecules and Ga, Ge, Cs, and Sb atoms, produce  $2 \times 2$  on Si(113) [15,21–24], the atomic structure of adsorbate-induced Si(113) $2 \times 2$  has been studied extensively. Recently, it comes to be conclusive that the atomic structure of adsorbate-induced Si(113) $2 \times 2$  is composed of two atomic chains of adatoms and tetramers (or pentamers), aligned along  $[1\bar{1}0]$  and alternatively arranged along  $[3\bar{3}2]$ , while Sb adatom and Si tetramer chains (Fig. 3(b)) were suggested to be preferable on  $2 \times 2$ -Sb [22]. For this reason, we suggested that the S1'–S2' and S3' bands originate from the Sb adatom and Si tetramer chains, respectively, in comparison with the energy bands of Cs/Si(111) $2 \times 2$  and Sb/Si(111) $1 \times 1$  [18]. Since each surface band of  $2 \times 5$ -Sb has a one-to-one analogous band on  $2 \times 2$ -Sb, it is persuasive that the S1–S2 and S3 bands of  $2 \times 5$ -Sb may be due to the Sb adatom and Si tetramer chains, respectively.

The existence of common building blocks could be supported by Heringdorf et al.'s STM experiments of H/Si(113) [15]. Firstly, we need to understand how hydrogen atoms on Si(113) provide sequential phase transitions through H/Si(113) $2 \times n$  ( $n = 13, 7, 5,$  and  $2$ ) [15]. The STM images of H/Si(113) $2 \times n$  are composed of two common chains, a 'bean-like' chain and a double linear chain aligned along  $[1\bar{1}0]$  which were interpreted as due to the H/Si(113) $2 \times 2$  structure and its domain wall, respectively, [15]. A competing interaction between the 'bean-like' chain and the double linear chain produces various  $\times n$  across the chain direction ( $[3\bar{3}2]$ ) [15]. The 'bean-like' chain, arranged uniformly on H/Si(113) $2 \times 2$  [15], could be assigned as due to the tetramer (or the pentamer) chains in comparison with other adsorbate-induced Si(113) $2 \times 2$  [22,23]. The H/Si(113) surface also produces a  $2 \times 5$  phase with two possible configurations: one 'bean-like' chain + two double linear chains and two 'bean-like' chains + one double linear chain in the  $2 \times 5$  unit cell [15]. Similarly, Müssig et al.'s STM experiments [22] show that the  $2 \times 2$ -Sb structure and its domain wall make local  $2 \times 5$ -Sb in the STM image of  $2 \times 2$ -Sb, which is not mentioned in the report. From the analogy of STM images between H/Si(113) and Sb/Si(113), we suggest that the  $2 \times 5$ -Sb structures could be built up of the  $2 \times 2$ -Sb structure and its domain wall, as shown in Fig. 4(c) and (d). The atomic structure model with a smaller domain wall (Fig. 4(c)) is more persuasive because the BW's of the surface bands of  $2 \times 5$ -Sb along  $[3\bar{3}2]$  are similar with those of  $2 \times 2$ -Sb and a wider domain wall results in a smaller BW along  $[3\bar{3}2]$ .

#### 4. Conclusions

ARPES experiments reveal Sb/Si(113) $2 \times 5$  to have three surface bands with BE's of 0.6, 1.08, and 1.64 eV at  $\bar{\Gamma}$ . Besides, the three surface bands were observed to have anisotropic 2D characteristics, where one of them is close to a quasi-1D band. The number of surface bands of  $2 \times 5$ -Sb and their band dispersions are quite similar with those of  $2 \times 2$ -Sb. This indicates that  $2 \times 5$ -Sb and  $2 \times 2$ -Sb have common building blocks, where  $2 \times 2$ -Sb is composed of Sb adatom and Si tetramer chains. We, thus, suggest tentatively that  $2 \times 5$ -Sb is built up of the  $2 \times 2$ -Sb structure and its domain wall, which could be also supported by the STM experiments of H/Si(113) and Sb/Si(113) [15,22]. Nevertheless, we do not exclude that a  $2 \times 5$ -Sb structure does not share a common building block with the  $2 \times 2$ -Sb structure, so that we also suggest tentative atomic structure models of  $2 \times 5$ -Sb based on the bulk-terminated Si(113) $1 \times 1$  structure.

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#### References

- [1] P. Segovia, D. Purdie, M. Hengsberger, Y. Baer, *Nature* 402 (1999) 504.
- [2] H.W. Yeom, S. Taketa, E. Rotenberg, I. Matsuda, K. Horikoshi, J. Schaefer, C.M. Lee, S.D. Kevan, T. Ohta, T. Nagao, S. Hasegawa, *Phys. Rev. Lett.* 82 (1999) 4898.
- [3] J.R. Ahn, J.H. Byun, H. Koh, E. Rotenberg, S.D. Kevan, H.W. Yeom, *Phys. Rev. Lett.* 93 (2004) 106401.
- [4] J.R. Ahn, H.W. Yeom, H.S. Yoon, I.-W. Lyo, *Phys. Rev. Lett.* 91 (2003) 196403.
- [5] P. Gambardella, A. Dallmeyer, K. Maiti, M.C. Malagoli, W. Eberhardt, K. Kern, C. Carbone, *Nature* 93 (2004) 077203.
- [6] J.R. Ahn, N.D. Kim, S.S. Lee, K.D. Lee, B.D. Yu, D. Jeon, K. Kong, J.W. Chung, *Europhys. Lett.* 57 (2002) 859.
- [7] R. Losio, K.N. Altmann, A. Kirakosian, J.-L. Lin, D.Y. Petrovykh, F.J. Himpsel, *Phys. Rev. Lett.* 86 (2001) 4632.
- [8] J.N. Crain, A. Kirakosian, K.N. Altmann, C. Brombergre, S.C. Erwin, J.L. McChesney, J.-L. Lin, F.J. Himpsel, *Phys. Rev. Lett.* 90 (2003) 176805.
- [9] G. Grüner, *Density Waves in Solids*, Addison-Wesley, Massachusetts, 1994.
- [10] N.F. Mott, *Metal-Insulator Transitions*, Taylor and Francis, New York, 1990.
- [11] P. Bak, *Rep. Prog. Phys.* 45 (1982) 587.
- [12] M. Hupalo, J. Schmalian, M.C. Tringides, *Phys. Rev. Lett.* 90 (2003) 216106.
- [13] J.Z. Wang, J.F. Jia, X. Liu, W.D. Chen, Q.K. Xue, *Phys. Rev. B* 65 (2002) 235303.
- [14] W.W. Pai, J.E. Reutt-Robey, *Phys. Rev. B* 53 (1996) 15997.
- [15] F.-J. Meyer zu Heringdorf, H. Goldbach, H.-L. Günter, M. Horn-von Hoegen, V. Dorna, U. Köhler, M. Henzler, *Surf. Sci.* 458 (2000) 147.
- [16] K.-S. An, C.C. Hwang, C.Y. Park, A. Kakizaki, *Jpn. J. Appl. Phys.* 39 (2000) 2771.
- [17] K.-S. An, C.C. Hwang, H.S. Kim, C.Y. Park, I. Matsuda, H.W. Yeom, S. Suga, A. Kakizaki, *Surf. Sci.* 478 (2001) 123.
- [18] K.-S. An, J.R. Ahn, Y.K. Kim, E.S. Cho, C.Y. Park, C.C. Hwang, T. Okuda, *Surf. Sci.* 583 (2005) 199.
- [19] K.-S. An, C.C. Hwang, R.J. Park, J.B. Lee, J.S. Kim, C.Y. Park, S.B. Lee, A. Kimura, A. Kakizaki, *Jpn. J. Appl. Phys.* 36 (1997) 2833.
- [20] K.-S. An, C.C. Hwang, Y.K. Kim, E.S. Cho, C.-Y. Park, S. Pukird, A. Kakizaki, T. Okuda, T. Kinoshita, *Surf. Sci.* 513 (2002) 49.
- [21] K.-S. An, C.C. Hwang, C.Y. Park, N. Kamakura, A. Kimura, A. Kakizaki, S. Suga, *J. Electron. Spectrosc.* 88–91 (1998) 701.
- [22] H.-J. Müssig, J. Dabrowski, W. Arabczyk, S. Hinrich, G. Wolff, *J. Vac. Sci. Technol. B* 14 (1996) 982.
- [23] Z. Zhang, K. Sumitomo, H. Omi, T. Ogino, *Phys. Rev. Lett.* 88 (2002) 256101.
- [24] H. Suzuki, H. Nakahara, S. Miyata, A. Ichimiya, *Surf. Sci.* 166 (2001) 166.