One-dimensional electronic structure of the Sb-decorated Si(1 1 3)2 × 2 surface

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Abstract

Various adsorbates prefer commonly 2 × 2 translational symmetry on Si(113), whose structure models were suggested to be composed of one-dimensional (1D) atomic chains, aligned along [1 1 0], of adatoms and tetramers (or pentamers). We characterized clearly the electronic structures of the 1D chains using the Sb-decorated Si(113)2 × 2 surface. The 1D chains on Sb/Si(113)2 × 2 were found to produce three energy bands with binding energies of 1.0, 1.4, and 1.75 eV at the normal emission by angle-resolved photoemission spectroscopy experiments. The three bands show interesting dimensional characters; the two energy bands with binding energies of 1.0 and 1.4 eV are close to ideal 1D ones in comparison with the other close to a quasi 1D one. In this report, we will describe the 1D energy bands on the bases of the 1D atomic chains.

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1. Introduction

The fabrications of one-dimensional (1D) structures have been recently encouraged to study the exotic phenomena of 1D electron systems such as the Luttinger liquid and the Peierls instability.
The Luttinger liquid was reported on the Au and Si atomic chains of Au/Si(557) [1] and on single-walled carbon nanotubes [2]. In addition, 1D charge density waves due to the Peierls instability were found on the Indium atomic chains of In/Si(111) [3,4] and on the Au and Si atomic chains of the Au-decorated stepped Si surfaces [5]. Other fascinating 1D ground states were also reported. The Na-Si atomic chains of Na/Si(111) were suggested to form a 1D Mott-Hubbard insulator which is expected to have a 1D antiferromagnetic order [6] and the Co atomic chains of Co/Pt(557) were found to show 1D ferromagnetism [7].

Among several techniques for the fabrications of 1D structures, self-assemblies are appropriate to prepare a wide range of 1D structures. In general, the self-assemblies require 1D templates with high anisotropy. The anisotropy is provided basically by the intrinsic structure natures of flat surfaces such as the Si-dimer chains on Si(100) which have been used for the 1D growths of molecules [9,8]. Besides, the extrinsic stepped structures also provide the anisotropy, as observed on those of the nearly-isotropic Si(111) surface [5], where Au decorations on the stepped Si(111) surfaces result in the formations of Au and Si atomic chains deviating from the flat Si(111) structure.

The 1D template with intrinsic anisotropy is applicable to the high-index Si(113) surface. The high-index Si(113) surface has its intrinsic flat reconstructed $3 \times 2$ surface without a stepped or a faceted structure [10], where, usually, high-index surfaces become stable by driving facets of low-index surfaces. Although the structure models of Si(113)$3 \times 2$ are still conflicting [11–13], the models are composed of common building blocks such as adatoms (A), tetramers (T) based on dimers (D) without interstitials (I) (just tetramers hereafter), and tetramers with interstitials (pentramers (P) hereafter); two representative models are called the oppositely-puckered (OP) [13] (see Fig. 1(a) and the adatom-dimer-interstitial (ADI) [12] (see Fig. 1(b)) models, respectively. In both models, the tetramers (or pentamers) and adatoms are located alternatively along both $[1\bar{1}0]$ and $[\bar{3}3\bar{2}]$, where a 1D electron system cannot be expected.

For this reason, the 1D growths reported on Si(113) [14,15] may be based on the intrinsic anisotropy of the unreconstructed Si(113)$1 \times 1$ structure rather than one of the reconstructed $3 \times 2$ structure.

The building blocks of Si(113)$3 \times 2$ have been proposed to rearrange, as due to various adsorbates, in order to have $2 \times 2$ translational symmetry by scanning tunneling microscopy (STM) experiments and theoretical calculations, as shown in Fig. 1(c) and (d) [16,17]. The structure models of the $2 \times 2$ phase are built up of the 1D adatom and tetramer (or pentramer) chains aligned along $[1\bar{1}0]$ [16,17]. This may originate basically from the relief of strain which is generated by Si-adsorbate bonds interacting with the intrinsic anisotropy of the unreconstructed Si(113)$1 \times 1$ [16,17]. Up to now, the expected 1D energy bands of the 1D chains have not been measured clearly especially for their dispersions along $([1\bar{1}0])$ and across $([\bar{3}3\bar{2}])$ the chain direction.

Fig. 1. Atomic structures of (a) the Wang et al.’s [13] oppositely-puckered (OP) and (b) the Dabrowski et al.’s [12] adatom-dimer-interstitial (ADI) models of Si(113)$3 \times 2$, (c) the Wolff and co-workers [17] adatom-tetramer (AT) model of Sb/Si(113)$2 \times 2$, and (d) the Zhang et al.’s [16] adatom-pentramer (AP) model of Ge/Si(113)$2 \times 2$. 

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In this report, we clarified the energy bands of the 1D chains on Sb/Si(113)2×2 along both [110] and [332], where the adatoms and tetramers are replaced by the Sb adatoms and Si tetramers, respectively, as shown in Fig. 1(c). The three bands of the 1D chains were found to be more dispersive along [110] than along [332], as expected from the structures of the 1D chains. In addition to the anisotropy of the dispersions, the three bands show interesting dimensional natures: the band structure is composed of both a quasi and two ideal 1D bands. We suggest that the ideal and quasi 1D bands originate from the Si-adatom and Sb-tetramer chains, respectively, which will be discussed in detail in the following.

2. Experimental

The photoemission measurements were performed at the beamline BL-18A of Photon Factory, High Energy Accelerator Research Organization (KEK) [18]. The nominal energy and angle resolutions were better than 150 meV and 1°, respectively. Energy bands were measured using two photon energies of 21.2 and 11 eV. The clean Si(113)3×2 surface was prepared by the repeated cycles of annealing at 900 °C and subsequent flashing at 1200 °C, as confirmed by low energy electron diffraction (LEED) patterns with clear non-integer spots. Sb atoms were deposited using quartz crucibles, and relative Sb coverage ($h_{\text{Sb}}$) was calibrated from the intensity ratio of Sb3d and Si2p spectra.

3. Results

Various adsorbates such as H2 molecules and Ga, Ge, Cs, and Sb atoms have produced commonly the 2×2 phase [16,17,19,15,20], which impresses the 2×2 phase with a key structure in understanding the interactions of adsorbates with Si(113), as studied for Si(111)3×1. Fig. 2 shows the $\theta_{\text{Sb}}$ dependence of valence bands at the normal emission on the annealed Si(113) surface at 600 °C [21]. The clean Si(113)3×2 phase is known well to show two surface bands (S8 and S9) with binding energies (BE’s) of 1.1 and 2.0 eV, respectively, and three bulk bands (B1, B2, and B3) at the normal-emission valence band [18]. As increasing $\theta_{\text{Sb}}$, the clean 3×2 surface is changed sequentially into 1×n, 2×5, and 2×2 phases, which is consistent with our previous LEED experiments [22]. Consequently, the bulk bands are bent toward the lower binding energy side. Before the formation of the 2×5 phase, two surface bands (S6 and S7) with BE’s of 0.9 and 1.47 eV, respectively, grow accompanied by the reduction of S8. At higher $\theta_{\text{Sb}}$, the 2×5 and 2×2 phases show their surface bands; two surface bands (S4 and S5) with BE’s of 0.75 and 1.7 eV, respectively, on the 2×5 phase and three surface bands (S1, S2, and S3) with BE’s
of 1.0, 1.4, and 1.75 eV, respectively, and one surface resonance (SR) band with a BE of 3.7 eV on the 2 × 2 phase.

In order to figure out the dimensional characters of the three bands of Sb/Si(113)2 × 2, their dispersions along [110] and [332] were measured using a photon energy of 11 eV, as shown in Fig. 3 (along chains) and Fig. 4 (across chains). Along [110] (the chain direction in Fig. 1), the S1–S3 bands are highly dispersive with band widths (BW) of 0.85, 0.40, and 0.72 eV, respectively. Here, the BW of S2 was not measured accurately because of its existence at a limited k-space (see Fig. 3) but is at least 0.40 eV. In comparison, the S1–S3 bands are relatively flat across the chain direction ([332]). In addition, the BW’s ≈ 0.1 eV of S1 and S2 deviate remarkably from the BW = 0.41 eV of S3 (see Fig. 4). From those results, we reach the conclusion that the 1D chains of Sb/Si(113)2 × 2 are electronically 1D and, in detail, show the coexistence of quasi (S3) and ideal (S1 and S2) 1D electronic structures.

The dimensional characters of the three bands of Sb/Si(113)2 × 2 are quite similar with the well-defined 1D electronic structure of In atomic chains on In/Si(111)4 × 1 with two quasi and one ideal 1D bands [4]. As discussed thoroughly for the In atomic chains, a quasi 1D band and ‘an ideal 1D band’ indicate whether a corresponding 1D chain interacts with the neighbor identical chains through the energy band: only the quasi 1D bands contribute to a ordering across the In chain direction. In comparison with the In atomic chains, the Si(113)2 × 2 structure are composed of two kinds of atomic chains, i.e. the adatom and tetramer
bands may originate from the Sb-adatom chains, related to the adatom. Therefore, the S1 and S2 bands are expected to be located at the normal emission although three bands were not mentioned explicitly on Sb/Si(113) [17]. The difference between the tetramer and the pentamer may be due to surface strain depending on the existence of the interstitial, and the tetrarsers and pentamers become stable energetically by puckering themselves on both models. Up to now, the various Si(113)2 × 2 surfaces have been expected to have the common structure, as discussed for the common structure of the various Si(111)3 × 1 surfaces [23].

Based on the common structure of Si(113)2 × 2, the origins of the S1–S3 bands are narrowed down into the Sb adatoms and Si tetrarsers. Here, we need to introduce the previous ARPES experiments on Si(113) to trace the origins further. The energy bands of the 2 × 2 phase were studied only on Cs/Si(113), where three bands were measured obviously at the normal emission although their dispersions along [1 10 ] and [3 3 2] were not explicit [20]. The three bands of Cs/Si(113)2 × 2 are located at BE’s of 0.7 (S1’), 1.0 (S2’), and 1.7 eV (S3’), respectively. Interestingly, the S3’ band of Cs/Si(113)2 × 2 has the same BE with the S3 band of Sb/Si(113)2 × 2, while both the S1’ and the S2’ bands are shifted by 0.3 eV toward the lower binding energy side in comparison with the S1 and S2 bands. These results provide important clues in figuring out the origins of the S1–S3 bands. As known well on Si(111)3 × 1, the adsorption site is independent of adsorbates and is thus unique [23]. This implicates that Cs and Sb atoms on Si(113)2 × 2 are expected to be located at the same adatom site. For these reasons, the change of an adsorbate means the replacement of the adatom, which consequently influences energy bands related to the adatom. Therefore, the S1 and S2 bands may originate from the Sb-adatom chains, and the S3 band may be due to the Si-tetramer chains.

In addition, the energy bands of Sb/Si(113)1 × 1 provide more information for the origins, where all dangling bonds of the unreconstructed Si(113)1 × 1 are saturated completely by Sb adatoms [21]. In this case, the Sb adatoms form 1D chains aligned along [1 1 0] which resembles the Sb-adatom chains on Sb/Si(113)2 × 2. The single surface (SS) band of Sb/Si(113)1 × 1 is located at the same BE of 1.0 eV at the normal emission with the S1 band of Sb/Si(113)2 × 2. Moreover, the SS band has a similar dimension character with the S1 and S2 bands of Sb/Si(113)2 × 2: the SS band is dispersive (BW = 0.7 eV) along [1 1 0] and is flat (BW = 0.2 eV) along [3 3 2]. These similarities also support that the S1 and S2 bands originate from the Sb-adatom chains, where the bigger BW of SS than those of S1 and S2 along [3 3 2] may be because of the smaller distance between the Sb-adatom chains on Sb/Si(113)1 × 1 [21].

The remaining question is “Is it possible that the Sb-adatom chains on Sb/Si(113)2 × 2 produce the two (S1 and S2) bands rather than a single band expected usually and observed on Sb/Si(113)1 × 1?” There is a possible explanation if the two bands truly come from the Sb-adatom chains. The Sb-adatom chains with the ×1 periodicity along the chain direction could be disturbed by the Si-tetramer chains with the ×2 periodicity. This makes the Sb1 and Sb2 adatoms in Fig. 1(c) become nonidentical, which consequently induces Jahn-Teller-type [16,24] double periodic lattice distortion (PLD) on the Sb-adatom chains. The Jahn-Teller-type distortion on the Ge-adatom chains of Ge/Si(113)2 × 2 was found obviously from STM experiments and discussed thoroughly [16], where a charge transfer between nonidentical Ge1 and Ge2 adatoms in Fig. 1(d) occurs. Meanwhile, the Jahn-teller-type distortion can be also noticed from the previous STM images on Sb/Si(113)2 × 2, but was not mentioned explicitly on the original report [17]. Therefore, we suggest that the Jahn-Teller-type double PLD could split degenerate bands due to the Sb adatoms into the two (S1 and S2) bands to further lower a total energy.
4. Conclusions

The 1D atomic chains of Sb/Si(1 1 3)2 × 2 were studied by ARPES experiments. The two chains of Sb adatoms and Si tetramers were found to produce three 1D energy bands with interesting dimensional characters; S1, S2, and S3 with BE’s of 1.0, 1.4, and 1.75 eV, respectively. We suggest that the two (S1 and S2) ideal 1D bands originate from the Sb-adatom chains undergoing the Jahn-Teller-type double PLD and the one (S3) quasi 1D band is due to the puckered Si-tetramer chains. This will shed lights on studies for the common 2×2 structure with the 1D chains on Si(1 1 3). Further theoretical calculations for the energy bands will be required to understand in detail their origins and the coexistence of the quasi and ideal 1D bands.

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