High-resolution photoemission spectroscopy study of the single-domain Si(110)-16×2 surface

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(Received 26 December 2006; published 12 March 2007)

We have investigated the valence band structure and Si 2p photoemission spectra of the single-domain Si(110)-16×2 surface with higher resolution than previous studies. We found that the highest occupied surface state, reported to be dispersive in the previous studies, is resolved into the two surface states with flat energy dispersions. This reveals that the two surface states are not produced by Si π-bonded chains, as suggested in the previous studies, but originate from the building blocks with spatially localized electronic structures such as a Si tetramer and a Si adatom. Si 2p line shapes show directly five surface components without any curve fitting. Various atomic structure models, especially the adatom-tetramer-interstitial model, of the Si(110)-16×2 surface are considered to figure out the atomistic origins of the surface components and states.

DOI: 10.1103/PhysRevB.75.125309 PACS number(s): 68.35.Rh, 73.20.−r, 79.60.−i

I. INTRODUCTION

The understanding of geometric and electronic structures of reconstructed low-index Si surfaces has been essential for characterizing various adsorbate-induced surface reconstructions and for widening their applications. Among reconstructed low-index Si surfaces, Si(100)-2×1, Si(111)-7×7, and Si(110)-16×2, only the Si(110)-16×2 surface is still not well understood.1,2 Furthermore, recently the interests for the Si(110) surface have continued to grow because of its potential applications. First, complementary metal-oxide semiconductor transistors, based on Si(110) wafers, were found to have better hole mobility than ones based on Si(100) wafers.3 Second, the anisotropic structure of the Si(110) surface has been used as a template to grow nanowires.4 Third, Si nanowires with small diameters were reported to grow along the [110] direction, having a hexagonal cross section of the (110) face and bounded by {111} and {100} facets.5,6

Despite such growing interests, the atomic structure of the Si(110)-16×2 surface is not established mainly because it is as complex as the Si(111)-7×7 surface.1,2 Morphological studies reported that up-and-down terraces alternating regularly on the surface play a major role to maintain the long-range 16×2 reconstruction.2,7,9 In particular, the arrangement of “pairs of pentagons,” observed by scanning tunneling microscopy (STM), has been considered as a cornerstone in constructing its atomic structure model.10,11 In order to explain such observations, several atomic structure models have been suggested, based on building blocks such as π-bonded chains, adatoms, tetramers, regular steps, and missing rows: stretched-hexagon adatom,12 tetramer-interstitial,10 five-membered adcluster,11 and adatom-tetramer-interstitial (ATI) models [see Fig. 1(c)].1

Recently, Stekolnikov et al. proposed that the most stable structure for the long-range 16×2 reconstruction can be produced by combining the ATI configuration with the regular step arrangement.2 This reveals tetramers to donate electrons to adjacent adatoms, which reproduces well the pentagonal arrays of spot shapes in the STM images.2

In comparison to morphological studies, high-resolution electronic information of the Si(100)-16×2 surface has been relatively rare in figuring out the long-range 16×2 reconstruction and testing its atomic structure models.1 Cricenti et al. first reported the Si 2p spectra13 and energy bands14 of the Si(110)-16×2 surface, which gives an overall electronic insight for the surface. However, the insufficient energy reso-

FIG. 1. (a) The LEED pattern of the clean Si(110)-16×2 surface and (b) 1×1 surface Brillouin zone. The schematic of the Stekolnikov et al. adatom-tetramer-interstitial model in (c) illustrates the sequence of pentagons and adatoms (the hatched circles) on up-and-down terraces. The pentagon consists of a tetramer atom (the filled circle), a first-layer atom (the open circle), and an interstitial atom located at its center (the small open circle). The dotted box indicates the unit cell of the 16×2 surface. Chains with (without) small open circles are the first-layer (second-layer) atoms.
lutions in the photoemission spectroscopy (PES) experiments prohibit observing accurate electronic information. Thus, the surface components of the Si 2p spectra were not decomposed directly from their line shapes, which provides uncertainty for the number of surface components and their binding energies. Moreover, the insufficient energy resolution makes it difficult to define dispersions of energy bands, and a double-domain Si(110)-16 × 2 surface, used in the experiments, limits the determination of accurate energy bands along symmetric directions.

In this paper, we measured extensively the high-resolution valence band structure and Si 2p photoemission spectra of the single-domain Si(110)-16 × 2 surface. The present valence band spectra reveal two surface states to locate at binding energies below 1 eV and to have flat energy dispersions along all symmetric directions. This suggests that the atomic structure of the Si(110)-16 × 2 surface should consist of building blocks with spatially localized electronic structures. Moreover, the surface components of the Si 2p photoemission spectra were directly resolved from their line shapes measured at various emission angles and photon energies. This makes it possible to determine obviously the number of surface components and their binding energies. Most of the photoemission spectral features are well explained by the Stekolnikov et al. ATI model with regular steps arrangement among various atomic structure models.

II. EXPERIMENT

The photoemission measurements were performed at two different locations. Si 2p core-level photoemission spectra were measured at a soft x-ray beamline (BL-8A1) connected to an undulator of the synchrotron radiation source at the Pohang Light Source (PAL) in Korea. The endstation is equipped with a high-resolution electron analyzer (SES-2002, Gamma Data, Sweden). The overall instrumental energy resolution, defined by photon beam and electron analyzer, is better than 40 meV and the acceptance angle of the analyzer is ±8°. The Si 2p core-level photoemission spectra were taken at 90 K in order to enhance the resolution by reducing the thermal broadening and were analyzed by a standard nonlinear-least-squares fitting procedure using Voigt functions. Angle-resolved photoemission spectra were measured with a photon energy (hν) of 90 eV and the energy-distribution curve mode, using an undulator synchrotron radiation at the beamline 7.0.1.2 of the Advanced Light Source (ALS) and a high-resolution electron energy analyzer (SES-100, Gamma Data, Sweden). The nominal energy and angular resolutions were better than 15 meV and 0.15°, respectively. The well-ordered Si(110) surface was prepared by repeated cycles of flashing at 1200 °C and subsequent annealing at 700 °C. This procedure produced a well-defined 16 × 2 LEED pattern, as shown in Fig. 1(a).7

III. RESULTS AND DISCUSSION

A. Angle-resolved photoemission spectroscopy

The valence band spectra of the clean Si(110)-16 × 2 surface were extensively measured. Representative valence band spectra along the three symmetry directions, [001], [110], and [110], are shown in Figs. 2 and 3. No discernible photoemission intensity is observed from the Fermi energy to the binding energy of 0.2 eV. This indicates that the clean Si(100)-16 × 2 surface is semiconducting, which is consistent with the Stekolnikov et al. theoretical calculations.2 The valence band spectra show various different spectral features with large and small dispersions. In the valence band spectra along Γ-X’, four energy bands, S1, S2, U1, and U2, are found to be nearly flat with bandwidths below 0.2 eV, while other two energy bands, B1 and B2, are dispersive with bandwidths at least larger than 2 eV. The flat energy dispersion is one of characteristic features of surface bands, as observed on the Si(111)-7 × 7 surface,13 and the S1 and S2 bands are located within the bulk-band gap. For these reasons, the S1 and S2 bands can be assigned as surface bands with E0’s of 0.4 and 0.9 eV, respectively. Other two dispersive bands, B1 and B2, are located within the projected bulk bands and are consistent with bulk bands observed in the previous studies.16 We thus assign the B1 and B2 bands as bulk ones. The S1 and S2 surface bands were also noticed along other symmetric directions, Γ-M and Γ-X, and were also found to be flat. The U1 and U2 bands, observed along the Γ-X’ and Γ-M directions, and the U3 band, observed along the Γ-X direction have flat energy dispersions, but are located within the projected bulk bands. It is thus not obvious whether the U1, U2, and U3 bands are
The ATI model is based on the “pairs of pentagon” and alternative raised and lowered strips. It reproduces well the characteristic features of STM images, structure models is the most stable structure in energetics and with the large 16 hexagon adatom, 12 tetramer-interstitial,10 five-membered adcluster,11 and ATI models1 have been suggested, which are known state is denoted by $E_b$. In order to speculate on atomistic origins of the surface bands and in building up an atomic structure model, the flat energy dispersions of the surface bands reveal the $S_1$ and $S_2$ bands not to originate from the $\pi$-bonded chain. The $S_1$ and $S_2$ bands could be rather due to building blocks with spatially localized electronic structures such as the tetramers, adatoms, and unsaturated $\pi$-bonded chains near step edges of the ATI model. The filled-state STM image taken at a bias voltage of ~1.0 V exhibits only the tetramers and adatoms in the unit cell, which is reproduced by theoretical calculations based on the ATI model.2,10 This leads to the conclusion that the $S_1$ and $S_2$ bands with $E_b$’s below $1 \text{ eV}$ are related to the tetramers and adatoms. In the ATI model, charge is transferred from the tetramers to the adatoms, so that the adatoms are expected to have a higher $E_b$ than the tetramers. This supports that the $S_1$ and $S_2$ bands are produced by the tetramers and adatoms, respectively.

The surface bands could be understood further by the resemblance of the Si(110)-16 × 2 surface with the Si(111)-7 × 7 surface. Both surfaces are stabilized by long-range reconstructions and total energies are lowered by charge transfers between adatoms and rest atoms on the Si(111)-7 × 7 surface and between tetramers and adatoms on the Si(110)-16 × 2 surface. The $E_b$’s and energy dispersions of the surface bands of the Si(111)-7 × 7 are also analogous to those of the Si(110)-16 × 2 surface.15 Two surface bands on the Si(111)-7 × 7 surface, originating from adatoms and rest atoms, respectively, are flat with bandwidths below $0.2 \text{ eV}$ and are located at $E_b$’s of 0.15 and 0.9 eV, respectively. The charge transfer from the adatoms to the rest atoms on the Si(111)-7 × 7 surface lowers the energy level of the rest atom. This also supports the assignments of the $S_1$ and $S_2$ surface bands of the Si(110)-16 × 2 surface as due to the tetramers and adatoms, respectively, based on the charge transfer from the tetramers to the adatoms.

**B. Si 2p core-level photoemission spectroscopy**

Figure 4 shows the Si 2p spectra of the clean Si(110)-16 × 2 surface measured at various $h\nu$’s and emiss-
The fitting procedure proves that the six components reproduce consistently all Si 2p core-level spectra measured at various $h\nu$’s and $\theta_e$’s, where representative fitting results are shown in Fig. 5. Here, the Gaussian and Lorentzian widths are 0.26 and 0.06 eV, respectively. The line shape and curve fitting analysis find obviously that the Si 2p core-level spectrum of the Si(110)-16×2 surface is composed of five surface components; the SCLS’s of the $SC_1$, $SC_2$, $SC_3$, $SC_4$, and $SC_5$ components are $-0.83$, $-0.33$, 0.26, 0.50, and 0.70 eV, respectively. In the previous studies, the number of surface components were determined only from the curve fitting analysis because of a lack of an energy resolution and their SCLS’s thus were not accurate. In comparison, the present Si 2p line shapes resolve conclusively the surface components and make it possible to determine accurately their SCLS’s.

To connect the building blocks of the atomic structure model of the Si(110)-16×2 surface with the surface components, we need to refer the previous assignments of the Si 2p core-level spectra of Si surfaces with well-established atomic structure models. The building blocks of the ATI model with distinctively different bonding characters from the bulk $sp^3$ bond are tetramers, interstitials, adatoms, and unsaturated $\pi$-bonded chains at step edges. We first consider the $SC_1$ and $SC_2$ components with negative SCLS’s of $-0.83$ and $-0.33$ eV, respectively. The rest atom on the Si(111)-7×7 surface and the $\pi$-bonded chains on the Si(111)-2×1 surface are known to produce surface components with negative SCLS’s of $-0.70$ and $-0.44$ eV, respectively. In the ATI model, Stekolnikov et al. show that charges are transferred from the tetramers to the adatoms. This indicates that the adatom with charge gain on the ATI model is similar to the rest atom on the Si(111)-7×7 surface. Additionally, a part of the underlying $\pi$-bonded chains at step edges are not saturated by tetramers or adatoms. The adatoms and unsaturated $\pi$-bonded chains thus could produce the $SC_1$ and $SC_2$ components. Second, we take the surface components, $SC_3$, $SC_4$, and $SC_5$, with positive SCLS’s into account. Among five surface components, the $SC_3$ component is the least surface sensitive, has the largest intensity, and is located near the $BC$ component, as shown in Fig. 5. This implies that the second-layer Si atoms could produce the $SC_3$ component, as observed on the Si(100)-2×1 and Si(111)-7×7 surfaces.15,20 The intensity of the $SC_4$ component is remarkably larger than other surface components except the $SC_3$ component. Thus, the underlying $\pi$-bonded chains, occupying the most surface atoms in the unit cell, could be the origin of the $SC_4$ component.15,20 The tetramers could also be one of the origins of the surface component with positive SCLS’s because the tetramers are positively charged due to the charge transfer from the tetramers to the adatoms. A part of the tetramer is expected to be involved in the charge transfer so that the actual number of Si atoms in the unit cell is below 16, where the number of underlying $\pi$-bonded chains in the unit cell is 52. When considering the intensity of the $SC_5$ component relative to those of other surface components, it is likely that the $SC_5$ component comes from a part of the tetramer.

IV. CONCLUSION

The single-domain Si(110)-16×2 surface has been studied by high-resolution angle-resolved and Si 2p core-level photoemission spectroscopy. In the valence band spectra, we identified two distinct surface states with $E_k$’s of 0.4 and 0.9 eV, respectively. The flat energy dispersions of the two
surface states imply that the Si(110)-16 × 2 structure is composed of building blocks with spatially localized electronic structures such as a tetramer and an adatom. We suggest that the two surface states with $E_b$'s of 0.4 and 0.9 eV originate from the tetramer with the interstitial and the adatom, respectively, based on the adatom-tetramer-interstitial model. Additionally, the high resolution Si 2$p$ spectra allow to resolve five surface components with SCLS's of $-0.83$, $-0.33$, $0.26$, $0.50$, and $0.70$ eV, respectively. Based on the ATI model, the five surface components with SCLS's may come from the underlying $\pi$-bonded chain at the step edge, while the $SC_4$ and $SC_5$ components with negative SCLS's may be due to the adatom and the unsaturated tetramer, respectively.

**Acknowledgments**

This work was supported by the Korea Research Foundation Grant funded by the Korean Government (MOEHRD) (Grant No. KRF-2006-312-C00120) and Korea Science Foundation through the SRC program (Center for Nanotubes and Nanostructured Composites) of MOST/KOSEF. One of the authors (J.R.A.) is also supported by the Korea Research Foundation Grant funded by the Korean Government (MOEHRD) (Grant No. KRF-2005-005-J11903). One of the authors (H.W.Y.) is supported by MOST through Center for Atomic Wires and Layers of the CRI program. The Advanced Light Source is operated under DOE contract at Lawrence Berkeley National Laboratory.

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