Surface Science 632 (2015) L13–L17

Contents lists available at ScienceDirect

Surface Science

journal homepage: www.elsevier.com/locate/susc

Surface Science Letters

Si(100)-2 × 1-H dimer rows contrast inversion in low-temperature scanning tunneling microscope images

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ARTICLE INFO

Article history:
Received 24 July 2014
Accepted 27 October 2014
Available online 30 October 2014

Keywords:
LT-STM
Quantum transport
Si(100)-2 × 1-H
Contrast inversion
Atomic scale devices

ABSTRACT

Detailed low temperature scanning tunneling microscope images of the Si(100)-2 × 1-H surface show a remarkable contrast inversion between filled- and empty-state images where the hydrogen dimer rows appear bright for filled-state images and dark for empty-state images. This contrast inversion originates from the change in the dominant surface states and their coupling to the tip apex and the bulk silicon channels as a function of the bias voltage: dimer Si – Si bonding states dominate the filled-state images and valley states associated with Si – Si anti-bonding states dominate the empty-state images. Care is required when constructing and interpreting the atomic structure of dangling-bond structures on the Si(100)-2 × 1-H surface.

1. Introduction

The hydrogen-passivated Si(100)-2 × 1 surface is an important platform for the construction of atomic scale circuits [1,2] and molecule-based devices [3] since Si(100):H is a robust surface [4] with a low defect density [5] and a relatively large surface band gap of 2.1 eV [6]. The Si(100):H surface has therefore been studied extensively by low temperature ultrahigh vacuum scanning tunneling microscopy (LT-STM) [7–9]. Surface hydrogen atoms of the Si – Si dimer rows can be desorbed with atomic precision by pulsing the STM tip bias voltage to create surface dangling bonds. The surface dangling bonds introduce well-defined states in the Si(100):H surface band gap and have been proposed as building blocks for single atom transistors [2], quantum dots [10], quantum wells [11],and logic gates [12–14]. The atom-by-atom construction of dangling bond devices requires the precise location of the surface hydrogen atoms. As demonstrated in this letter, the STM contrast of the Si(100):H surface depends on the imaging conditions (bias voltage and tip structure) and does not always match the atomic scale structure of the Si(100):H surface. At positive bias voltage, the inter-dimer valleys appear brighter than the topologically higher dimer rows. This contrast inversion leads to an apparent half row shift of the surface atomic scale structure and highlights that the determination of the atomic scale structure of atomic wires and circuits constructed on the Si(100)-2 × 1-H surface using STM images needs to be done with care.

Contrast in STM images results from the electronic coupling between the tip apex and substrate bulk states through the surface states and depends on the number of bulk electronic channels as a function of the bias voltage. Therefore, it does not always represent the surface atomic scale structure or the surface local density of states (LDOS). A careful examination of published Si(100)-2 × 1-H STM images shows contrast inversion in some cases, especially when filled- and empty-state images are compared using dangling bond dimers [6] or reconstruction boundaries [15] as reference points. Depending on the bias voltage [16] and the tip apex to surface distance [17], STM images of the MoS_2 [18] and Mo_2S_3 [19] surface show either the surface S lattice or the sub-surface Mo lattice, or both. An apparent contrast inversion of the dimer rows between filled-state and empty-state images has also been observed on the clean Si(100) surface [20,21]. Also for filled- state images of the clean Si(100) surface, a bias dependent change in the apparent structure of the image was reported [22]. Tip-induced band bending (TIBB) is potentially an important effect in STM studies of semiconductor surfaces and depends strongly on the doping level, the tip-sample distance, as well as the tip structure [23–25].

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http://dx.doi.org/10.1016/j.susc.2014.10.016
0039-6028/

2. Experimental and computational methods

To analyze and elucidate the bias voltage and tip dependent contrast inversion of the Si(100)-2 × 1-H surface, STM images of a hydrogen-passivated Si(100) surface were recorded at liquid helium temperature (4 K) using a ultrahigh vacuum low temperature STM (Omicron Nanotechnology GmbH) with a base pressure of 2×10^{-10} mbar [26]. Si(100) samples were obtained from Sb-doped n-type wafers and B-doped p-type wafers both with a resistivity <0.1 Ω cm. The Si(100):H surface was prepared by annealing at 600 °C for 12 h and several cycles of flashing to 1200 °C for 10 s. After this, the substrate temperature was reduced to 375 °C and atomic hydrogen was dosed up to 13.4 L ($1\ L = 1 \times 10^{-6}$ Torr s) at a H_2 partial pressure of 2×10^{-8} mbar. The H_2 gas (>99.95% purity) was introduced via a leak valve and cracked by passing over a tungsten filament at 35 mA, about 15 cm above the sample.

STM images were computed using the surface Green-function matching (SGFM) method [27] with an extended Hückel molecular orbital (EHMO) Hamiltonian [28] tuned to match HSE06 density functional theory band structures [29]. The STM junction was modeled as a semi-infinite W(111) slab, a Si-terminated STM tip, a five-layer Si(100):H surface, and the semi-infinite Si(100) bulk, as illustrated in Fig. 3a.

3. Results and discussion

Fig. 1a–d shows STM images of n-type Si(100):H with a setpoint current of 20 pA and for a large range of bias voltages. The corresponding line-scan profiles perpendicular to the dimer rows are shown in Fig. 1e. The filled-state image (Fig. 1d) shows the 2 × 1 dimer rows with a maximum at the center of the Si dimer rows and a minimum at the inter-row valleys (Fig. 1d, e), matching the surface structure. The filled-state images are relatively insensitive to the change in bias voltage. A more interesting variation of the contrast with the bias voltage is observed for the empty-state images. At a low positive bias voltage (+1.0 V, Fig. 1c), the contrast is similar to the filled-state contrast and matches the surface geometry, except for the presence of a shallow local minimum instead of a maximum at the center of the dimer rows. When the bias voltage is increased, the local minimum at the inter-row valleys becomes shallower and at +1.3 V a fully symmetric 1 × 1 structure with equally spaced peaks is observed (Fig. 1b, e). For a bias voltage above +1.3 V, the 2 × 1 pattern re-emerges, however, the minimum is now at the center of the dimer rows and maximum is found at the center of inter-dimer valleys, a complete inversion of the contrast (Fig. 1a). The contrast inversion is more clearly shown in Fig. 2, recorded for p-type Si(100):H, where the bias was switched suddenly between −1.6 V and +1.6 V while scanning. The reversibility of the contrast inversion demonstrates that piezo creep or thermal drift does not cause the contrast inversion. Experiments performed with p-type Si(100):H demonstrate that the inversion is independent of the doping (see Supplementary Data, Section 1 for details).

The dI/dV spectra for both the n- and the p-type Si(100):H surface do not show signature peaks for surface dangling bond or defect states (see Supplementary Data, Section 2 for details), in agreement with previous spectra [6,30], suggesting that such states do not contribute to the contrast inversion. The effect of tip apex to sample distance on the image was explored as well. The contrast inversion in the empty-state images was also observed for a bias voltage of +1.8 V and setpoint currents between 400 and 500 pA, showing that the contrast inversion is observed for a small range of tip-sample distances (see Supplementary Data, Section 3 for details). Since the contrast inversion was observed for a range of tip-sample distances and both for n- and p-type samples, TIBB is unlikely a dominant factor in the observed effect.

To understand the origin of the observed contrast inversion, constant current images and T(E) electronic transmission spectra through the tunnel junction were computed for the STM junction shown in Fig. 3a. The calculated T(E) spectra are shown for two tip apex positions: at the center of the Si dimer rows (Fig. 3b, on dimer, dotted red curve) and at the center of the inter-dimer valleys (Fig. 3b, between dimers, blue curve). In the valence band region (filled states) and at the center of the dimers, T(E) is always higher than T(E) at the center of the valley, resulting in images which are bright above the dimer rows and darker above the valleys (Fig. 4e), in agreement with the experimental images.

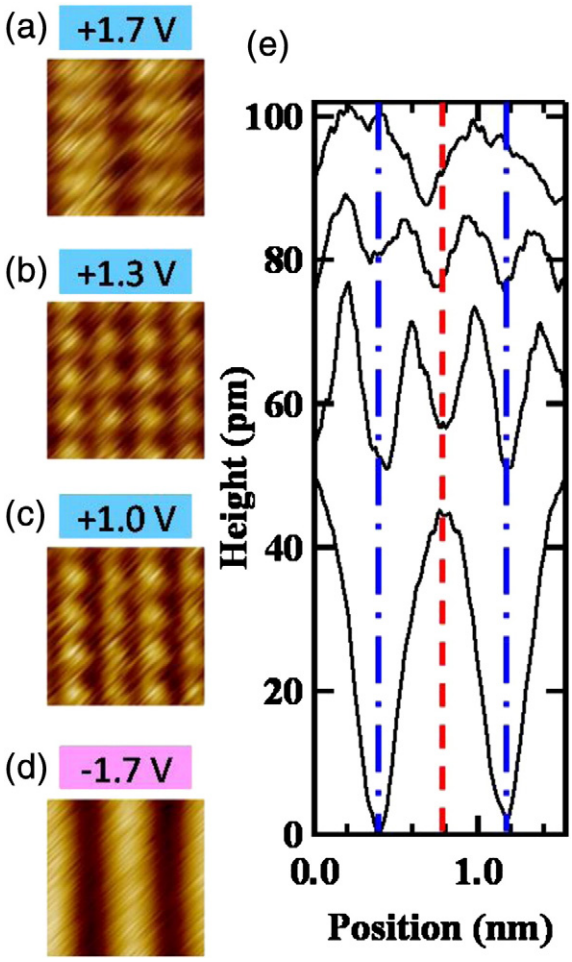

Fig. 1. (a)–(d) STM images of the n-type Si(100)-2 × 1-H surface for different bias voltages (20 pA current, 1.54 nm × 1.54 nm scan area). (e) Corrugation profiles perpendicular to dimer rows for the images in (a)–(d) from top to bottom. The minima and maxima in the corrugation are indicated to illustrate the contrast inversion.

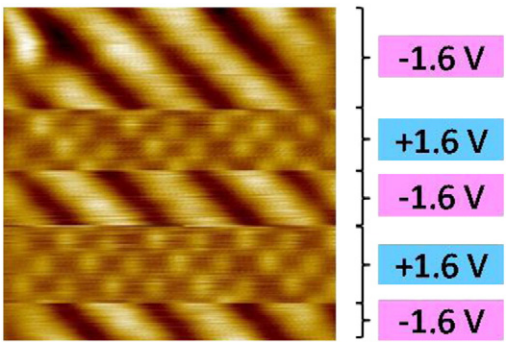

Fig. 2. STM image of p-type Si(100)-2 × 1-H. The bias voltage was suddenly switched from −1.6 V (filledstate) to +1.6 V (empty state) while scanning (20 pA current, 4 nm × 4 nm scan area).