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Surface Reconstruction of Pt/Si(001)

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ABSTRACT Platinum-induced surface reconstructions on Si(001) were investigated by scanning tunneling microscopy. The Si(001) surface shows $c(4 \times 6) + c(4 \times 2)$-type reconstruction after Pt hot deposition at 750 °C. The $c(4 \times 2)$ reconstruction is formed by regular arrangement of Pt ad-atoms at the hollow sites between two Si dimers on Si(001). The $c(4 \times 6)$ structure is formed by long-range ordering of Si dimers superimposed on the $c(4 \times 2)$ reconstruction. The surface reconstruction changes with the local Pt coverage and missing dimer density. An atomic model for $c(4 \times 6) + c(4 \times 2)$ is proposed based on the observed $c(4 \times 4)$ surface reconstruction, a new surface reconstruction, which is observed following a high-temperature anneal at 900 °C. The $c(4 \times 4)$ surface reconstruction is regular and ordered in both the dimer-row direction and the direction perpendicular to the dimer rows. The reconstruction is formed by the regular arrangement of Si dimers and Pt ad-atoms sitting on top of the hollow sites surrounded by two dimers. An atomic model for this new reconstruction is proposed.

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1 Introduction

Nanometer-scale low-dimensional structures have attracted great interest in recent years because of their potential usage as building blocks for nanoscale devices. These systems also exhibit interesting electronic, magnetic, and transport properties [1, 2]. The success of the rare-earth (RE = Er, Ho, Dy, Gd, and Sc) disilicide nanowire growth on Si(001) substrates [3–7] method opens a promising window for the fabrication of nanoscale devices by self-assembly. Kavanagh et al. found that Pt silicide can also form wire structures by using an in situ transmission electron microscopy study of Pt silicide growth on Si(100) substrates [8]. Compared with RE silicide nanowires, the Pt silicide nanowires have a lower aspect ratio, but better chemical stability. Moreover, Pt silicide is also broadly used as contact and interconnect material in Si-based electronic devices because of its low Schottky barrier to p-type Si in a range useful for infrared detector applications and low resistivity to n-type Si [9–14]. Therefore, Pt silicide is a promising material candidate for the nanodevice fabrication.

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However, low-coverage studies of Pt growth on Si(001) are limited: these studies are crucial for the nanodevice fabrication. Okada et al. [15] first observed the $c(4 \times 6) + c(4 \times 2)$ low-energy electron diffraction (LEED) pattern. Itoh et al. [16] later performed LEED and scanning tunneling microscopy (STM). Atomic models for $c(4 \times 2)$, which is formed by the regular arrangement of Pt atoms embedded on hollow sites surrounded by two Si dimers, and for $c(4 \times 6)$, which is formed by long-range ordering of missing dimer defects superimposed on the $c(4 \times 2)$ structure, were proposed in that paper. Choi et al. [17] performed LEED and ISS (ion scattering spectroscopy) and proposed that there is no missing dimer defect in the $c(4 \times 6)$ structure. The detailed atomic structure of surface reconstruction of Pt on (100) is still in debate. In the present study, we investigated the surface reconstruction of Pt on Si(001) by utilizing scanning tunneling microscopy.

2 Experiment

All experiments were performed in an ultra-high-vacuum (UHV) chamber with base pressure less than 2.0×10^{-10} Torr. The UHV system is equipped with an in situ Omicron VT-STM system. p-type Si(001) substrates were cleaned by the RCA method before insertion into the chamber. The clean Si(001)-2×1 reconstructed surface was prepared by flashing the sample at 1115 °C for 15 s after annealing at 600 °C for about 3 h. The cleanliness of the Si(100) surface was examined by STM, to confirm a clean Si(001)-2×1 reconstructed surface. The substrate was heated resistively and the temperature was measured by an infrared pyrometer. Pt was deposited on the Si substrate at 750 °C for 10 min with a flux of 0.02 ML/min by an Oxford e-beam gun and the substrate was post-annealed for an additional 5 min. The pressure during the deposition is less than 1.0×10^{-9} Torr. The flux was calibrated ex situ by the Rutherford backscattering technique and after cooling the surface was examined by the STM. The sample was subsequently annealed at 800 °C and 900 °C for 5 min. STM was performed after each annealing step. All STM measurements were carried out on constant tunneling current with the current setting of 0.1 nA at room temperature.

3 Result and discussion

The as-deposited surface and the annealed surface are composed of Pt-induced surface reconstruction and is-

lands. The properties of the islands will be discussed in another paper. In the present study, we will focus only on the surface reconstruction of the as-deposited surface and the annealed surface. The as-deposited surface shows a typical $c(4 \times 6) + c(4 \times 2)$ reconstruction pattern, while the annealed surface has a new reconstruction, $c(4 \times 4)$. Therefore, the discussion will be divided into two sections accordingly. In order to state the discussion clearly, the $c(4 \times 4)$ surface reconstruction will be discussed first.

3.1 $c(4 \times 4)$ *surface reconstruction*

After annealing the Pt/Si(001) surface at 900 °C for 5 min, a new surface reconstruction, $c(4 \times 4)$, not reported in the literature previously, emerges. Figure 1a shows the filled-state image of the reconstructed surface, which was taken at −2 V sample bias and 0.1 nA tunneling current. Figure 1b shows the corresponding empty-state image of the reconstructed surface, which was taken at +2 V sample bias and 0.1 nA tunneling current. Figure 1a and b were taken at the same region, but there is a small shift due to the thermal and mechanical drift. In Fig. 1a, there are two types of features clearly observed; one is a round ball-shaped feature and the other is a bright bean-shaped feature, referred to as *A* and *B*, respectively. The *A*-type features are well ordered in both the dimer-row direction and the direction perpendicular to the

dimer rows, while the *B*-type features are ordered only in the dimer-row direction. The dark feature in the filled-state image is attributed to the missing dimer defects by comparing with the empty-state images. Almost every bright *B*-type feature has a missing dimer defect accompanied either side along the dimer-row direction. The counterparts of the *A*- and *B*-type features in the filled-state images are labeled as *A′*- and *B′*-type features in the empty-state image. The *A′*-type feature in the empty-state image is made up of two-dimer like structure, in which four atoms can be seen forming a tetramer. The *B′*-type feature in the empty-state image looks like a single Si dimer, in which two atoms can be seen forming a dimer with brighter contrast than feature *A′*. Between every two *A′*-type features, there are one *B′*-type feature and one missing dimer without a preferred position order. The periodicity of the structure was examined to be four times the Si–Si atom distance (0.38 nm) within uncertainty. Then, the unit cells of the $c(4 \times 4)$ structure are assigned as the squares shown in Fig. 1a and b, respectively.

A simple model, ad-atom and Si-dimer model, is proposed in Fig. 1c, where the dashed circles are missing atoms and the dashed lines are the virtual bonds. Since Pt atoms are larger than Si atoms, steric constraint indicates that they are likely to sit on top of the hollow sites surrounded by two Si dimers rather than underneath, as in the case of C-induced (4×4) reconstruction [18]. The Pt atom and the four Si atoms
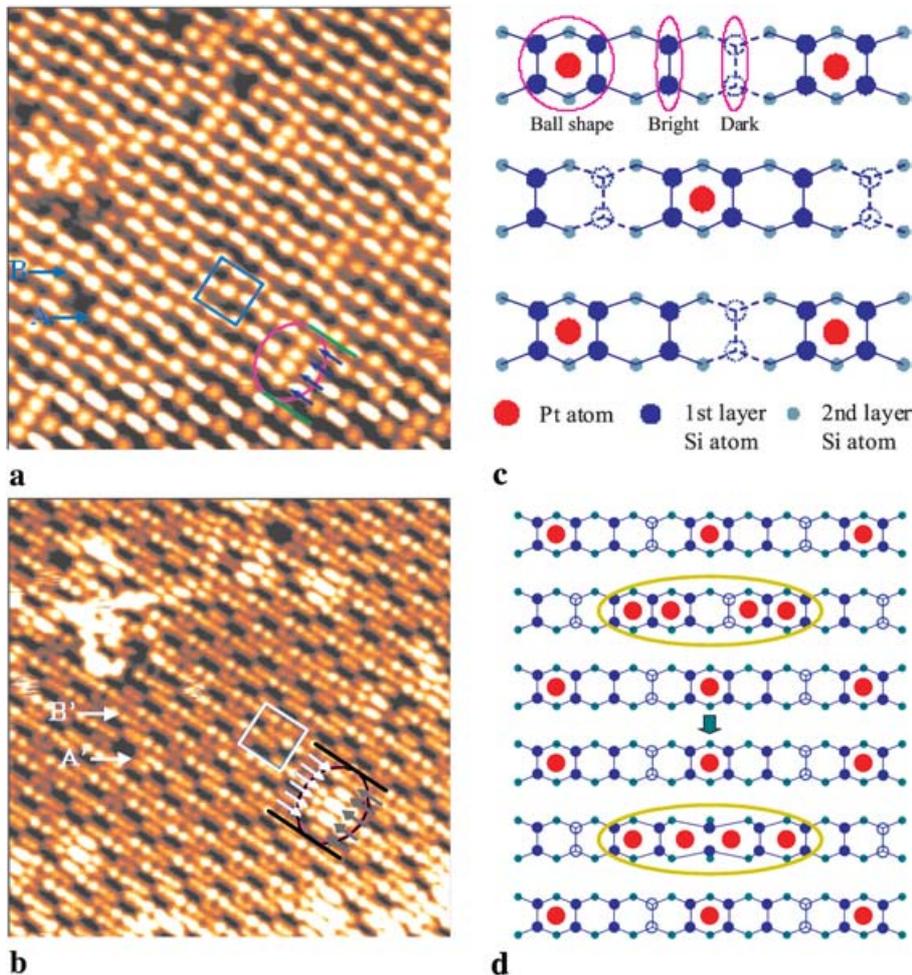
FIGURE 1   (**a**) Filled-state image of $c(4 \times 4)$ surface reconstruction. The image is taken at −2 V sample bias. The image size is 15 nm × 15 nm. (**b**) Empty-state image of $c(4 \times 4)$ surface reconstruction. The image is taken at +2 V sample bias. The image size is 15 nm × 15 nm. (**c**) Atomic model of $c(4 \times 4)$ surface reconstruction. (**d**) Schematic diagram of the defect structure in $c(4 \times 4)$ surface reconstruction

underneath correspond to the A- and A'-type features in the filled- and empty-state images, respectively. Because the surface electronic states of four Si atoms are passivated by the Pt atom sitting on top of them, they appear to be a round-shaped feature in the filled-state image and are resolved as four Si atoms in the empty-state image. Between two Pt atoms along the dimer-row direction, there is one dimer missing out of two dimers. The missing dimer appears dark. The remaining bare Si dimers correspond to the B- and B'-type features in the filled- and empty-state images, respectively. These dimers are bright in both the filled-state image and the empty-state image. The positions of bare Si-dimers are not fixed as shown in model since the two positions are equivalent and interchangeable, leading to the irregular zigzag pattern along the direction normal to dimer row in the filled state image.

In addition, there is one interesting defect feature worth noting, which is marked by an oval in Fig. 1a and b. There are four continuous A-type features in the filled-state image marked by blue arrows. Referring to the same location in the empty-state image, five Si-dimer-like features are marked by purple arrows and occupy six Si-dimer positions marked by blue arrows. According to the proposed model in Fig. 1c, there are three hollow positions which can hold Pt atoms between two nearby Pt atoms in the dimer-row direction. However, only two positions are occupied in the filled-state image. This discrepancy indicates that there are indeed only two deformed four-fold positions. Thus, the Si dimers between two adjacent Pt atoms along the dimer row may relax to lower the free energy when holding two more Pt atoms. The schematic is shown in Fig. 1d. This relaxation can be clearly seen in the empty-state image, where positions of the middle three of five dimer-like structures marked by purple arrows are shifted as indicated in Fig. 1d. Especially, the middle one is exactly shifted to the center position between two dimers. Therefore, this defect structure is consistent with the proposed atomic model of $c(4 \times 4)$ surface reconstruction and can be direct evidence for the model.

3.2 $c(4 \times 6) + c(4 \times 2)$ surface reconstruction

Figure 2a and b show the filled-state images of the Si surface after hot deposition at $750\,°C$, which were taken at -2 V sample bias and 0.1 nA tunneling current at different sample positions.

In Fig. 2a, there are both the $c(4 \times 6)$ and the $c(4 \times 2)$ unit cells, as marked by rectangles. There are the same features as the $c(4 \times 4)$ pattern, namely, the A-type ball-shaped feature and the B-type bean-shaped feature. By referring to the result of the $c(4 \times 4)$ pattern, the A-type ball-shaped feature is one Pt atom sitting on top of a Si tetramer, the B-type bean-shaped
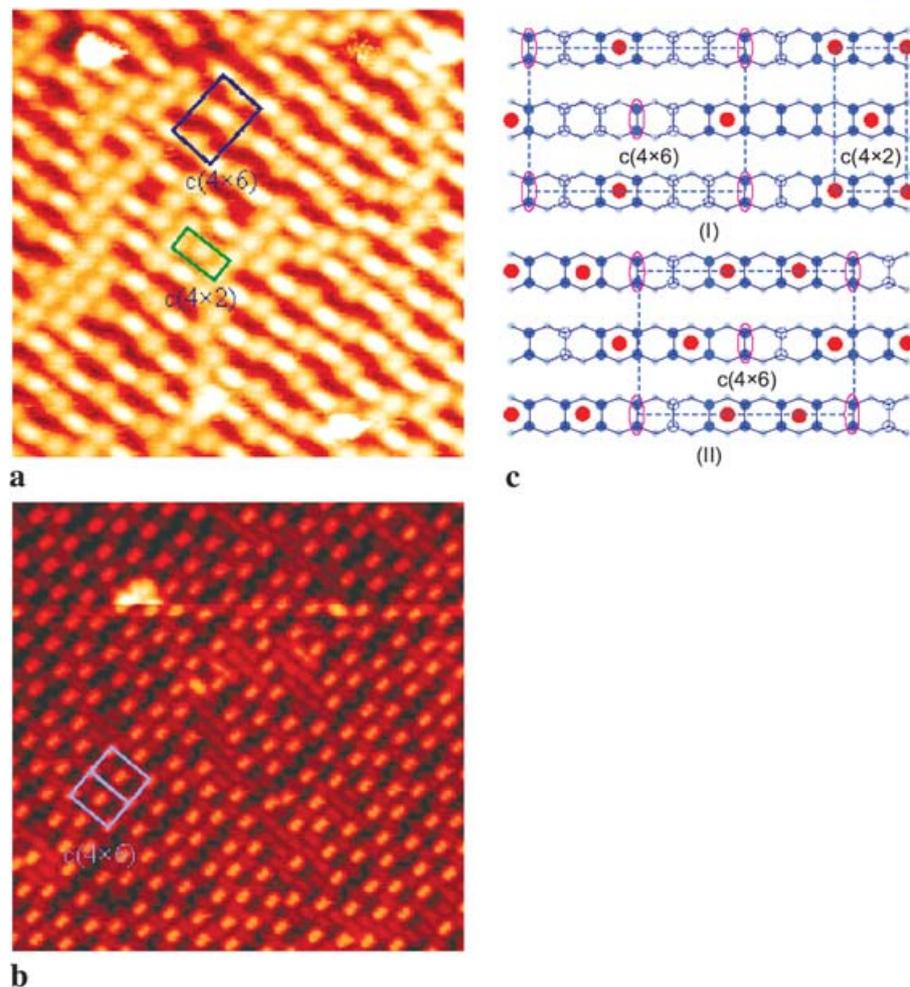
FIGURE 2 (a) Filled-state image of $c(4 \times 6)$ $+c(4 \times 2)$ surface reconstruction. The image is taken at -2 V sample bias. The image size is 11.25 nm × 11.25 nm. (b) Filled-state image of $c(4 \times 6) + c(4 \times 2)$ surface reconstruction. The image is taken at $+2$ V sample bias. The image size is 18.75 nm × 18.75 nm. (c) Atomic model of $c(4 \times 6) + c(4 \times 2)$ surface reconstruction

feature is the Si free dimer, and the dark region is the missing dimer. The image is not in agreement with the model proposed by Choi et al. [17], which claims no missing Si dimers presenting on the surface for $c(4 \times 6) + c(4 \times 2)$. Figure 2b has only a $c(4 \times 6)$ unit cell visible. There are still bean-shaped features accompanied by missing dimer defects on either or both sides along the dimer-row direction. The ball-shaped features are not visible and it seems that they formed a chain structure in the images. The reconstruction pattern is not regular, similar to what Itoh et al. observed [16]. The bright feature is aligned well in the dimer-row direction but not in the direction perpendicular to the dimer row.

One significant aspect is that the surface reconstruction varies in Fig. 2a and b. It can be seen from the images that the density of missing dimers is different, which could be caused by the variation of local coverage of Pt atoms. The atomic model for $c(4 \times 6) + c(4 \times 2)$ surface reconstruction given by Itoh et al. [16], however, is not compatible with the filled-state image in Fig. 2a. Thus, a modified atomic model for surface reconstructions $c(4 \times 6)$ and $c(4 \times 2)$ is given in Fig. 2c. Pt atoms are still located on the top of the hollow sites surrounded by two Si dimers. The $c(4 \times 6)$ structure is formed by the ordering of Si dimers superimposed on the $c(4 \times 2)$ structure when the Pt atoms are partially removed and missing dimer defects are introduced. Depending on how many Pt atoms are removed, there will be different $c(4 \times 6)$ surface reconstructions as shown in parts I and II of Fig. 2c.

4   Summary and conclusion

In conclusion, we have investigated the Pt/Si(001) interface by STM. The as-deposited Si(001) surface shows a $c(4 \times 6) + c(4 \times 2)$ reconstruction. The surface morphology depends on the local Pt coverage. After annealing at 900 °C, the surface reconstruction changes to perfect $c(4 \times 4)$. In all these three types of surface reconstructions, the Pt atoms are always sitting on top of the four-fold hollow site surrounded by two Si dimers. The $c(4 \times 6)$ structure is formed by the long-range ordering of Si dimers superimposed on the $c(4 \times 2)$ structure. The $c(4 \times 4)$ structure is formed by the regular arrangement of Pt ad-atoms and free dimers. Atomic models for these three structures are proposed. However, theoretical simulation of the surface reconstruction is necessary to verify the validity of the model. This part of the work will be done by our colleagues later.

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