Arrangement of the dimer structure on the Si(001)2x1 surface observed by low-temperature scanning tunneling microscope

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Abstract

Using a scanning tunneling microscope (STM) which can be operated under multiple extreme conditions of ultrahigh vacuum ($> 6 \times 10^{-9}$Pa), low temperature (>2.8K), and magnetic field (<11T), we studied a behavior of silicon dimer structure on the Si(001) 2x1 surface. Asymmetric (buckled) dimer structure, locally forming either c(4x2) or p(2x2) periodicity, was observed with positive sample bias voltages, while most of the dimers looks symmetric with negative sample bias voltages. These observations suggest that the observed symmetric dimer structure in the filled state images is not intrinsic; neither static symmetric dimer nor flip-flopped asymmetric dimer, but a matter of STM imaging mechanism. It turns out that magnetic filed, up to 10T, applied perpendicularly to the surface in the both directions does not affect the STM imaging at 4.5K.

Key words: silicon surface; silicon dimer structure; Si(001)2x1; scanning tunneling microscopy
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On Si(001) surface [1], two surface silicon atoms making a bond in the $< 110 >$ direction in order to reduce the number of dangling bonds, a dimer structure is formed. The dimers are arranged linearly in the $< 1\bar{1}0 >$ direction to form a so-called "dimer row" structure with a long range ordering of 2x1 periodicity. The unique feature that makes the surface quite interesting is that the dimer can be buckled, that is, one of the two dimer-composing atoms protruding further from the surface than the other. In the dimer-row direction, the asymmetric "buckled" dimer exhibits an "anti-ferromagnetic"-like interaction with the neighboring dimers, making a zigzag structure. Between the neighboring dimer-rows interaction can be either "ferromagnetic" or "anti-ferromagnetic", producing p(2x2) or c(4x2) ordering, respectively. A flip-flop motion of the buckled dimer is induced by thermal activation or by a proximity effect of the probe tip in scanning tunneling microscope (STM), but the motion is pinched off near local defects, such as steps and missing dimers.

Lots of theoretical and experimental studies using various techniques, including STM [2] [3] [4], have been performed [1]. Generally accepted scenario on the structure says that an order-disorder phase transition occurs at around 140K; below the transition temperature, the buckled dimers are arranged in an ordered manner with a periodicity of c(4x2), and above the temperature the thermally activated dimer flip-flop motion exhibits the 2x1 ordering [5]. Recently, Kondo et al.[6] reported an STM image taken below the transition temperature but showing non-buckled dimers, claiming an existence of new ground state structure different from the accepted scenario. Yokoyama and Takayanagi, then, showed an evidence of c(4x2) structure at low temperature from an analysis of electronic structure obtained by STM [7]. Since they also observed non-buckled dimer images with STM, they claim anomalous flip-flop dimer motion at low temperature (5K). Before their observations, Shigekawa et al. [8] demonstrated buckled-dimer STM images below the transition temperature, but there is still a doubt on the sample temperature [6].

In order to solve the undetermined situation, we carried out STM experiments at low temperature (4.5K).

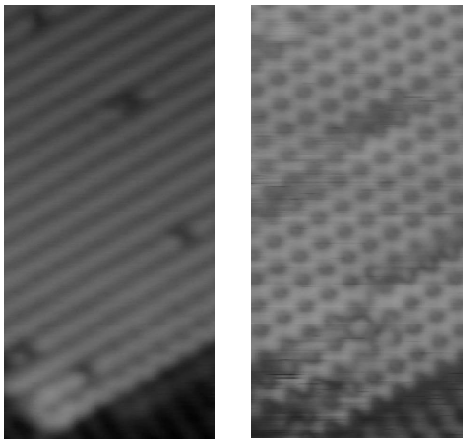

Fig. 1. STM images taken on the same area at 4.5K with a negative (left) and positive (right) sample bias voltage. The observed area is 14 nm x 7nm. The sample bias voltage and tunneling current is -1.47 V and 42pA (left), 1.51V and 42pA (right), respectively.

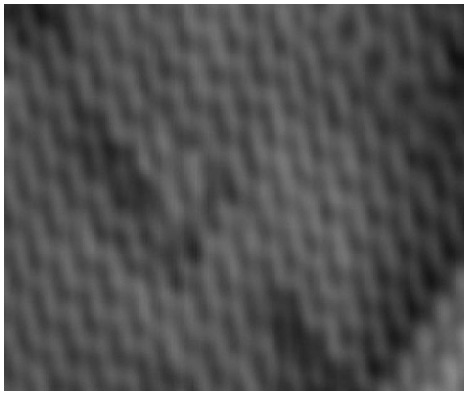

Fig. 2. STM image taken at 47K with a negative sample bias voltage. The size of the observed area is 10nm x 8.5nm. The sample bias voltage and tunneling current is -2.03V and 68pA.

Our results shows non-buckled images with positive sample voltages (filled state images). But, with negative sample voltages (empty state images), buckled dimer structure is clearly observed. These observations suggest an existence of asymmetric dimer structure at the low temperature and that apparent symmetric dimer structure in the filled state images is due to some STM imaging mechanism.

In the present study, we used a commercial STM setup made by Unisoku (USM type). The base pressure in the STM chamber is about 6×10^{-9}Pa. The Si(001)2x1 surface was prepared in a standard method; a small piece of silicon wafer (n-type, Sb-doped, 0.014-0.005 ohm·cm) was loaded into a UHV chamber. In the chamber, it was flashed at 120 $^\circ$C to make a clean surface with pressure lower than 2×10^{-8}Pa. Its cleanness was checked by STM observation. It turns out that the defect density is $\sim$2%.

Figure 1 shows STM images taken on same area with negative (left) and positive (right) sample bias voltages. Filled state and empty state of the sample are imaged, respectively. The filled state image shows many linear features running parallel each other. These are dimer-row structures with some missing dimers. You may find some segments showing a zigzag pattern in particular near defects and step edges. These are due to buckled dimers arranged in an "anti-ferromagnetic" manner along the dimer-row direction. The other area, which covers most of the imaged area, apparently looks having non-buckled symmetric dimers. We took filled-state STM images with a bias voltage ranging from -3V to -1.3V, and non-buckled dimer structure was always observed on most of the surface. The empty state image of the same area, presented in the right of figure 1, shows remarkable differences from its counterpart filled state image. Almost all area including one with a zigzag pattern in the filled state image shows a zigzag pattern, supporting a presence of buckled dimers on the surface. Applied bias voltage ranging from 3V to 1.6V does not affect basic feature of the dimer structure. Theoretical calculation [9] suggests the upper atom in the buckled dimer looks brighter (darker) in the filled (empty) state images.

Correlation of the zigzag pattern with a neighboring dimer row has two types: in phase and out of phase, which correspond to p(2x2) and c(4x2) structure, respectively. Occasionally, we observed a motion of the phase boundary and transitional fuzzy-looking regions as well in sequentially taken STM images, as was observed by Shigekawa et al. [8]. In spite of the motion, overall phase domain structure is kept in a series of empty-state imaging. It was not disturbed by an imaging of the filled state image showing non-buckling dimers. These images exclude a possibility of non-buckled -looking dimer imaging by flip-flop motion of dimers either thermally activated or tip induced. We conclude a formation of asymmetric dimer structure at the low temperature (4.5K) and speculated that symmetric dimer structure in the filled state images is due to STM imaging mechanism. But, the mechanism itself is not revealed yet, still under discussion.

One may think that the non-buckled dimmer in the filled state images are due to a limited spatial resolution. In fact, we also observed non-buckled dimer-like in the empty state images when its spatial resolution is low. In order to check this point, we took the filled state images at an elevated temperature, shown in figure 2. The image was taken with a sample temperature of 47K. Although it is a filled state image, it clearly shows buckled dimer structure, similar with those obtained at the liquid nitrogen temperature (77K) [3]. The observed non-buckled dimer image shown in figure 1 is not caused by a low resolution.

Theoretical calculation including an effect of spin

configuration in the dimer structure was reported by Artacho and Ynduráin [10]. According to their results, symmetric dimer with an anti-ferromagnetic spin arrangement is most stable. Although their result is not consistent with our experimental results, but it encourage us to observe the dimer structure under a magnetic field. The buckled dimer structure, by a charge transfer from the lower atom to the upper atom, is considered to have anti-parallel singlet spin configuration. Expecting a transition to symmetric dimer, which may have a magnetically-favored triplet spin configuration, we took several STM images under magnetic field up to 10T at 4.5K. We applied the field in the perpendicular direction to the surface, both upper and lower directions, but we could not find any significant changes in a structure and arrangement of dimer on the surface.

In conclusion, we studied a behavior of silicon dimer structure on the Si(001) 2x1 surface. Buckled dimer structure was observed in the empty state images, while in the filled state images most of the dimers looks symmetric. The observed symmetric dimer structure in the filled state images is due to neither static symmetric dimer nor flip-flopped asymmetric dimer, but a matter of STM imaging mechanism. We also found that magnetic filed, up to 10T, applied perpendicularly to the surface in the both directions does not affect the STM imaging at 4.5K.

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