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Tip-induced band bending on Sr/Si(100)-2×3 reconstructed surface

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Using Vary-temperature Scanning Tunnelling Microscopy (VT-STM), the geometric and electronic structures of technological important Sr/Si(100)-2×3 surface were investigated. Two important findings explained in this research. First, a phenomenon similar to quantum corral observed in the empty state STM image that near the bottom of the conduction band. This is aroused from the surface vacancies and phase boundary in the Sr/Si(100)-2×3 surface. And a new Sr/Si(100)-2×6 reconstructed structure coexist with Sr/Si(100)-2×3 surface has been prepared by accurately controlling the annealing temperature, both surface’s geometric structures can be described by dimer vacancy model. Second, tip-induced band bending phenomenon was observed in the Sr/Si(100)-2×3 surface at substrate temperature range from 76K to 300K. Experimental LDOS results from n and p-type silicon substrate confirms 0.3eV up the motion of the valence band minimum compare with bare Si(100)-2×1 surface. Buckled and unbuckled silicon dimer coexisting in the Sr/Si(100)-2×3 reconstructed surface contribute to the tip-induced band bending and energy band gap widen phenomenon. Which confirms that Sr atoms transfer electrons to the nearby silicon dimers, make the first layer silicon dimers kept at unbuckled state. © 2017 Author(s). All article content, except where otherwise noted, is licensed under a Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by/4.0/). https://doi.org/10.1063/1.4998918

I. INTRODUCTION

The shrinkage of the dimension of COMS device has led to higher gate leakage current. In order to reduce this, crystalline high k oxides, such as SrTiO₃, should replace the traditional gate oxide of SiO₂ and H₂O₂.¹⁻⁴ Owing to its high activity of surface silicon atom dangling bond, amorphous silicon oxide formed easily during the high-temperature growth process. This forbids the hetero-epitaxial growth of the SrTiO₃ thin film on silicon substrate. In order to resolve this issue, an important Sr/Si(100) buffer layer was introduced to saturate the silicon dangling bond, allowing the growth of crystalline SrTiO₃ on silicon substrate.⁵⁻¹⁰ The synthesis of novel functional crystalline oxide thin films on semiconductor substrates calls for atomic-level knowledge and controlling of the initial stages of the interface before hetero-junction formation.

In order to understand the electronic and geometric structures of this important Sr/Si reconstruction structures, surface sensitive techniques such as STM, RHEED, XPS and X-ray standing wave have been explored.¹¹⁻¹⁸ With the increase of Sr coverage on high-temperature Si substrate, Sr/Si(100)-2×3 was the first well-ordered reconstructed structure with Sr coverage of 1/6 monolayer, and Sr/Si(100)-2×1 was the second reconstructed structure with Sr coverage range

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from 1/4 to 1/2 monolayer. In the last decade, different geometric structures were proposed to explain the first well ordered Sr/Si(100)-2×3 reconstructed surface. Until recently, the dimer vacancy geometric model proposed by Reiner accepted by the science community. Theoretical calculations suggest insulator property of this surface, while experimental results suggest semiconductor property of this surface with energy band gap of 1.1 eV from STS at room temperature. Thus, detail investigation needed to understand the electronic structure of this important functional surface.

The geometric and electronic structures of Sr/Si(100)-2×3 surface were investigated using atomic resolution STM and STS at a different temperature. Tip-induced band bending phenomenon was found on this surface, which helped to deepen the understanding of this first well ordered stable reconstructed structure of Sr/Si(100) surface system.

II. EXPERIMENT

The experiments were performed in a home designed ultra-high vacuum system equipped with a low-temperature STM (MATRIX, Omicron GmbH) head with a base vacuum pressure of $2.0 \times 10^{-8}$ Pa. Two types of Si(100) wafers were used as substrates, one was a high resistivity p-type wafer (B-doped, 10 Ω·cm, Virginia Semi.), and the other was a low resistivity n-type wafer (As-doped, 0.005 Ω·cm, Virginia Semi.). We use the common flashing method to obtain Si (100)-2×1 reconstructed surface in ultra-high vacuum (UHV) condition. A pulsed laser deposition (PLD) technique was used to deposit a SrO ultra-thin film with a nominal thickness of 0.8 nm on the Si (100)-2×1 surface at room temperature. During deposition, the vacuum pressure was kept below 1 × 10^{-6} Pa, and the laser was introduced into the vacuum chamber via the quartz window. Ceramic SrO (Aldrich, 99.9%) target was prepared by sintering technique, the wavelength of the laser was 266 nm, the laser power was 1.5 W, and the deposition time was 15 s. After deposition, the sample transferred to the STM chamber in situ and annealed for 30 min at different setting temperature. During this process, the Oxygen atoms in the ultrathin SrO film will react with Si substrate, and forming volatile SiO above 800K, responsible for creating the atomic level flat Sr/Si (100) reconstructed surface. Both STM and STS measured at a temperature range between 76K and 300K using tungsten (W) tip.

III. RESULTS AND DISCUSSIONS

A. STM image of Sr/Si(100)-2×3 and Sr/Si(100)-2×3 coexist surface and their geometric structure

Fig. 1(a) show the typical large-scale Sr/Si(100)-2×3 STM image prepared by the above method. Our STM images have the same character similar to the results reported from Reiner and Kuzmin. Beside typical Sr/Si (100)-2×3 reconstructed surface, Sr/Si(100)-2×6 coexists in this area as shown in fig. 1(b), and the formation temperature of this surface is 850K. Figure 1(c) is an enlarged STM image of the Sr/Si(100)-2×6 reconstructed surface, showing that this structure has a symmetrical honeycomb structure. The geometric structure of this two surfaces can be described using model proposed by Reiner. Both Sr/Si (100)-2×3 and Sr/Si(100)-2×6 surfaces geometric structures were described using the same building block of dimer vacancy geometric model. Both reconstructed structures have buckled and unbuckled silicon dimer, as shown in Fig. 1(d) and Fig. 1(e). The main difference between the models is the Sr atom position in the respective unit cells, Sr atom shifts by half unit cell in the Sr/Si(100)-2×3 comparing with Sr/Si(100)-2×3. In fig. 1(c), we observe the direct half unit cell shift appear in the right part of high-resolution STM image.

B. Empty STM image of Sr/Si(100)-2×3 near the bottom of conductance band

After changing the bias polarity during scanning, we observed bias dependent STM image of Sr/Si(100)-2×3 surface which has the same character as reported by Du and J. H. He. Besides that, when we investigate STM image at the bias voltage near the bottom of conductance band, a new phenomenon emerges, as evident from fig. 2. In the magnified image of fig. 2(b) and fig. 2(d),
FIG. 1. STM images of Sr/Si(100)-2×3 and Sr/Si(100)-2×6 coexist surface on an n-type silicon substrate and plausible geometrical structures of these two reconstructed surfaces. Fig. 1(a) is the large area STM image of Sr/Si(100)-2×3 and Sr/Si(100)-2×6 coexist surface, with bias voltage of 1.5 V and tunneling current of 0.2 nA, 66.7×66.7 nm². Fig. (b) is the magnified picture of a selected area in Fig. 1(a) with same scanning condition. Fig. 1(c) is the high resolution Sr/Si(100)-2×6 STM image with bias voltage of 1.5 V and tunneling current of 20 pA. Fig. 1(d) is the geometric structure model of Sr/Si(100)-2×3. Fig. 1(e) is the geometric structure model of Sr/Si(100)-2×6. First layer silicon dimers are in the buckled state, while second layer silicon dimers are in the unbuckled state.

we can see that partial Sr/Si(100)-2×3 area displays a zigzag structure at the bias voltage of 0.8 V (empty state), whereas at the higher voltage of 1.3 V (empty state) it displays normal line structure. After investigating this area in detail, we propose two reasons to explain this phenomenon. First, the presence of surface vacancy defects around this area might be affecting the structure, as at least four such vacancies marked in fig. 2(d). Second is the contribution from phase boundary, one can easily distinguish this phase boundary transition from bright spots present in the left portion of fig. 2(b). The above two defects act like a quantum corral which is responsible for the behavior of Sr unit cell and silicon dimers displaying zigzag structure at a lower bias voltage of empty state STM images.

FIG. 2. is Empty state STM images of Sr/Si(100)-2×3 surface on an n-type silicon substrate with a formation temperature of 800 K. Fig. 2(a) is large scale with scanning condition of 0.8 V, 10 pA and 40×40 nm². Fig. 2(b) is enlarged the image of the selected area in fig. 2(a). Fig. 2(c) is the same area of Fig. 2(a) with different scanning condition of 1.3 V, 10 pA and 40×40 nm². Fig. 2(d) is the same area of Fig. 2(b) with a bias voltage of 1.3 V.
C. Electronic structure of Sr/Si(100) surface at a different temperature

1. The electronic structure of Sr/Si(100) on different type of silicon substrate

Since we used two types of the silicon substrate in our experiments, we want to know if there have any difference in electronic structure. So we collect the I-V curves and get \((\text{DI/} \text{DV})/\text{(I/V)}\) curve which represents the density of states near the Fermi level of the surface state. One common feature appearing in the empty state STS for both n-type and p-type silicon substrates, as indicated in the figure 3(b) and (c), compared with bare Si(100)-2×1 surface 0.3eV peak shift appearing in both spectra. This indicates that after Sr adsorb on the Si(100)-2×1 surface at high temperature (around 800K), Sr will donate its electrons to the nearby silicon dimer and forming stable Sr/Si(100)-2×3 reconstructed surface. As first layer silicon dimers will accept the transferred electrons, this dimer will change from the buckled state to the unbuckled state in one unit cell. Besides that, different type silicon substrates have different STS features at the filled state range, the STS of the n-type silicon substrate has prominent -1.7 eV peak, indicating strong back bond from third layer silicon atoms; while the STS of the p-type silicon substrate has prominent -0.8eV peak, indicating strong dangling bond from first and second layer silicon dimers.

2. Tip-induced band bending phenomena on Sr/Si(100)-2×3 surface

Since there exist buckled and unbuckled silicon dimers in Sr/Si(100)-2×3 surface, in order to understand the electronic structure further, we measured the STS of this surface at different sample temperature.

At room temperature, for high conductivity n-type silicon substrate (0.005Ω·cm) as shown in fig. 4(a), the energy band gap is decreased with increasing tunneling current from 10pA to 200pA (keeping bias voltage constant at 2.0V) as the distance between tip and sample shrink. Similarly, for p-type silicon substrate (10 Ω·cm) as shown in fig. 4(b), the energy band gap is also decreased with the increase of bias voltage from 1.6V to 2.4V (keeping tunneling current constant at 100pA), as the distance between the tip and sample shrink. This proved that the electronic property of Sr/Si(100)-2×3 behave same for both n or p-type silicon substrate at room temperature. The energy band gap widened from 0.71eV to 1.17eV for N-type silicon substrate, and from 0.69 to 0.87eV for P-type silicon substrate separately.

Due to the high resistivity of the p-type Sr/Si(100)-2×3 sample, we only investigated low resistive n-type samples at lower temperatures, that is 76K and 160K, the results are shown in fig. 4(c) and Fig. 4(d).

At 160K, a tunneling current was kept constant at 50pA while increasing the sample bias from -1.5V to -3.0V, which resulted in the increase in energy bandgap, with the filled state near Fermi level.

FIG. 3. Room temperature STS of Sr/Si(100)-2×3 surface with a different type of silicon substrate. Figure 3(a) is the STM image of typical Sr/Si(100)-2×3 and Si(100)-2×1 coexist surface on an n-type silicon substrate, which used to collect I-V curves, the scanning condition was -1.5V and 0.1nA. Figure 3(b) is STS of Sr/Si(100)-2×3 on an n-type silicon substrate, and Figure 3(c) is the STS of Sr/Si(100)-2×3 surface on a p-type silicon substrate.
FIG. 4. STS of Sr/Si(100)-2×3 surface at different substrate temperature. Fig. 4(a) is room temperature STS of n-type silicon. Fig. 4(b) is room temperature STS of p-type silicon. Fig. 4(c) is STS measured at 160K of n-type silicon. Fig. 4(d) is STS measured at 76K of n-type silicon.

changed from -1.08eV to -1.42eV. As seen in figure 4c the surface energy band gap is increased with the increase in tip-substrate distance. The energy band gap widened from 0.62eV to 1.22eV at 160K, which means the energy band gap widened about 0.6eV.

As sample temperature decreased to 76K, the conductivity further decreases, and the STS measurements have to be done at a relatively high bias voltage of -3.0V. From fig. 4(d) it is evident that at a lower temperature of 76K, the same phenomenon was observed as the energy band gap changed from 0.74eV to about 1.22eV, which means the energy band gap widened about 0.48eV. The surface state near the energy band gap became weak compared with the room temperature and 160K samples. It can be seen that the widest energy band gap of Sr/Si(100)-2×3 was around 1.2eV for an n-type silicon substrate with temperature range from 76K to 300K.

Electronic geometric structure in the above description proves that Sr/Si(100)-2×3 surface have tip-induced band bending property, as silicon dimers present in this Sr induced Si(100)-2×3. Which is similar to tip-induced band bending for Si(100)-2×1 surface as described in many kinds of literature.25–28 Here, we compare the band bending results of Sr/Si(100)-2×3 with n-type Si(100) 2×1 surface reported by K. Sagisaka.28 K. Sagisaka found that when the set current rose from 0.1 to 5.0 nA, the amount of energy shift in the position of the first filled state peak was approximately 0.3 eV, whereas the first empty peak shift by nearly 0.6 eV. The observed energy shifts were due to band bending induced by the tip electric field on Si(100)-2×1 surface. The difference between Sr/Si(100)-2×3
and Si(100)- 2×1 is that the former behave widen energy band gap phenomenon, while the latter behave narrower energy band gap phenomenon. This proves that silicon dimers dominate the electronic structure of Sr/Si(100)-2×3 surface, and Sr atom donates an electron to the nearby silicon dimer, thus forming buckled and unbuckled dimers.

IV. CONCLUSIONS

Using STM and STS, we investigated the geometric and electronic structures of Sr/Si(100)-2×3 reconstructed surface. Dimer vacancy model accurately describes the geometric model of Sr/Si(100)- 2×3 and Sr/Si(100)-2×6 reconstructed surfaces, and a phenomenon similar to quantum corral was observed in the empty state STM image, near the bottom conduction band. After investigating the STS of Sr/Si(100)-2×3 surface from temperature range between 76 and 300K, tip-induced band bending phenomenon was observed on both n-type and p-type silicon substrate. Besides that, 0.3eV peak up shift at empty state was observed from the STS on both n and p-type silicon substrate. Besides that, 0.3eV peak up shift at empty state was observed from the STS on both n and p-type silicon substrate. This confirmed that silicon dimer dominates the electronic structure of Sr/Si(100)-2×3 surface and Sr atoms contribute to the formation of unbuckled silicon dimers as the charge transfer happened.

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