The One-dimensional Property of Sr/Si(111)-3×2 Reconstructed Surface

Wenhan DU[a], Jingjing YANG, Yu ZHAO, Chao XIONG, Jin XIAO, Jinxiang MA and Xifang ZHU
Changzhou Institute of Technology, ChangZhou, JiangSu Province, China
[a]duwh@czu.cn, [1]

Abstract. The electronic and geometric structures of Sr/Si surface were investigated by Scanning Tunneling Microscopy. One-dimensional(1D) atomic concerted motion phenomenon was observed on this surface. Three reasons contribute to this phenomenon: First, low metal coverage of 1/6 monolayer with low energy occupation sites; second, weak interaction between Sr and Si substrate; third, surface vacancy formed in the high temperature annealing process and thermal fluctuation energy at room temperature. This findings lead to the conclusions that (3x2) reconstruction of Sr/Si system behave typical one-dimensional diffusion property at room temperature.

1. Introduction

Sr/Si reconstruction surface play an important role in the growth of high k oxides, such as SrTiO3 on Si substrate in semiconductor industry to reduce gate leakage current with the CMOS device dimension decreasing.

Different reconstruction structures, such as (2×3)Sr/Si and (2×1)Sr/Si have been reported for the Si(100) substrate, and plausible reconstruction structures have been proposed[1-10]. As for Si(111) substrate, when Sr atoms adsorbed on this surface, (3x2)-Sr/Si(111) reconstruction structure has been observed[7]. However we noticed that 1×3 spots in the LEED pattern was observed, and 3x2 spots was weak. What arouse this contradiction ,there are still lack plausible explanations.

Here , we use STM and STS to investigate (3x2)-Sr/Si(111) surface, and propose the plausible reason to compensate the difference between STM and LEED patterns.

2. Experiment

The experiments were performed in an ultra-high vacuum system with base pressure of 4.0×10^{-8} Pa, and equipped with a VT STM (MATRIX, Omicron GmbH). High resistive p-type Si(111) wafers were used as substrates. A pulsed laser deposition (PLD) technique

* Corresponding author: duwh@czu.cn,

was used to deposit SrO ultra-thin film with nominal thickness of 1.0nm on Si(111)-7×7 substrate at room temperature. After deposition, the sample was annealed at 700℃ for about 1h, during this process the O atoms in the SrO will react with Si and forming volatile SiO[8], thus leaving Sr/Si(111) reconstruction structure. Scanning tunneling microscopy measurements were performed at room temperature (RT).

3. Results and Discussions

3.1Geometric Structure of Sr/Si(111)-3x2 Surface

In the large scale STM image which shown in fig.1 (a), it can be noticed that Sr/Si(111)-3x2 surface reconstructed well ordered. A selected area were shown in the fig.1 (b), in this high resolution image two type atom rows appear: One was clear rows with atomic resolution, the other was blur rows with different length. The clear rows is characterized by a 3x2 unit cell (parallelogram) with a $3a_0$ between the neighboring rows and $2a_0$-period along the rows, here a_0=3.84Å is the lattice constant of Si(111). For clarified whether the Sr/Si(111)-3x2 surface has bias polarity dependence or not, we measured high resolution STM image shown in fig.1(c), during the measurement we change the bias polarity twice to identify the difference between filled state and empty state images. We observed one prominent circle protrusion appearing in the empty state image of 1.5V, and two protrusions appearing in the filled state of -1.5V in one unit cell. The bright protrusion in the empty state was situated in the middle of two protrusions in filled state image.

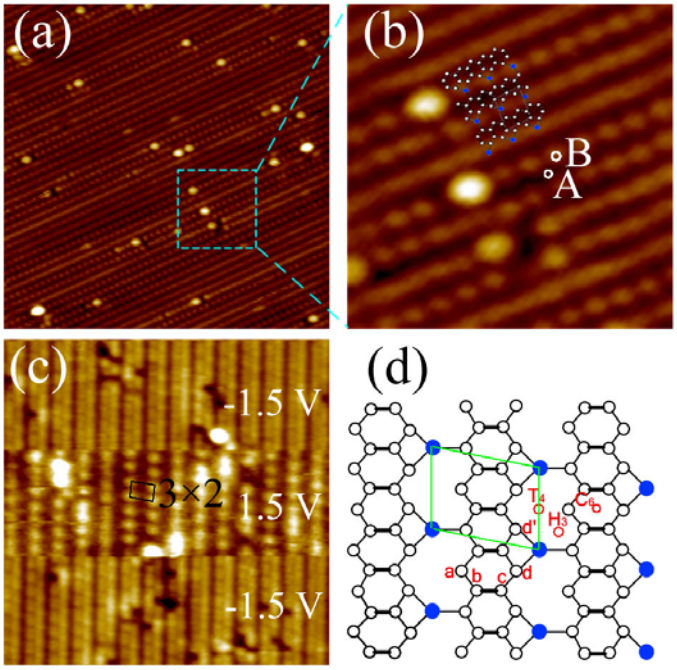

Fig.1 (a) Sr/Si(111)-3x2 surface with condition of V_{bias}=3.5V I_{set}=20pA 40×40nm^2. (b) Enlarge STM image from (a), 10×10nm^2. (c) High resolution dual bias STM image, ±1.5V and tunneling current of 10pA, 15×15nm^2. (d) HCC model proposed for Sr/Si(111)-3x2 surface.

Comparing our experimental STM images with theoretical results report by Lee[6], *et al*, we propose that the Sr/Si(111)-3x2 surface may be describe by the HCC model, which have been used to described other AEM atoms such as Ca and Ba induced Si(111)-3x2, fig.1(d) shows the model proposed for Sr/Si(111)-3x2 surface. The bright area in the empty state image at 1.5V reflect the Sr atoms position, while the double rows in the filled state image reflect the information of reconstructed Si atoms. Comparing with AE atoms induced Si(111)-3×1 surface, the (3×1) reconstruction of substrate silicon have some deformation, as indicated by the ellipse in the fig.1(c), the silicon atoms reacted with Sr atoms which denote as d and d' in the model have dimeric phenomenon, in the filled state image of fig.1(c) we observe this phenomenon.

3.2 1D Diffusion of Sr Atom Chains in Sr/Si(111)-3x2surface and its Origin

We measured two empty STM images of same area within 3min, and shown in fig.2(a) and fig.2(b), fig.2(c) was the subtraction image. After compare these two images we find that two typical changes appearing, as shown in fig.2(d): For the first type, bright rows behave obvious displacement, and the change length was varied from several (line1, 4, and line 10) to dozens of atoms (line3 and line6); for the second type, the atom rows in one image was clear, in the other image these clear rows become blurry, and the atom row length was also varied. Besides these two type changes, there also have two type rows behave no changes: one was clear atom rows, the other was blurry atom rows. In the total image, half atom rows change, and left part kept the initial state. The above phenomenon support Sr atoms behave motion in the room temperature. And we will give our explanations in the following part.

First, there exist Sr atom vacancy defects in the Sr/Si(111)-3x2 surface, Sr atoms nearby may move across these vacancy defects by the thermal fluctuation energy at room temperature , the selected change atom rows in fig.2(d) support this point.

Another factor comes from the lower coverage of 1/6 monolayer for Sr atoms. As Si substrate adopt the 3×1 reconstruction in HCC structure, there has only one Sr atom in a 3x2 unit cell, as two T4 sites in one unit cell have the same adsorption energy, when there have two metal atoms, the static electric force between them push the atoms away, thus these Sr atoms behave 1D motion phenomenon in the silicon channel.

Third, when measuring STM images, STM tip induced electric effect will accelerates the 1D chain motion. Besides, thermal energy at room temperature leads to the above 1D motion, which behave as the vacancy motion, and the change of atom line length in the filled state image. In the atomic resolution empty state image we can even observe Sr atoms moving along the silicon dimer row .

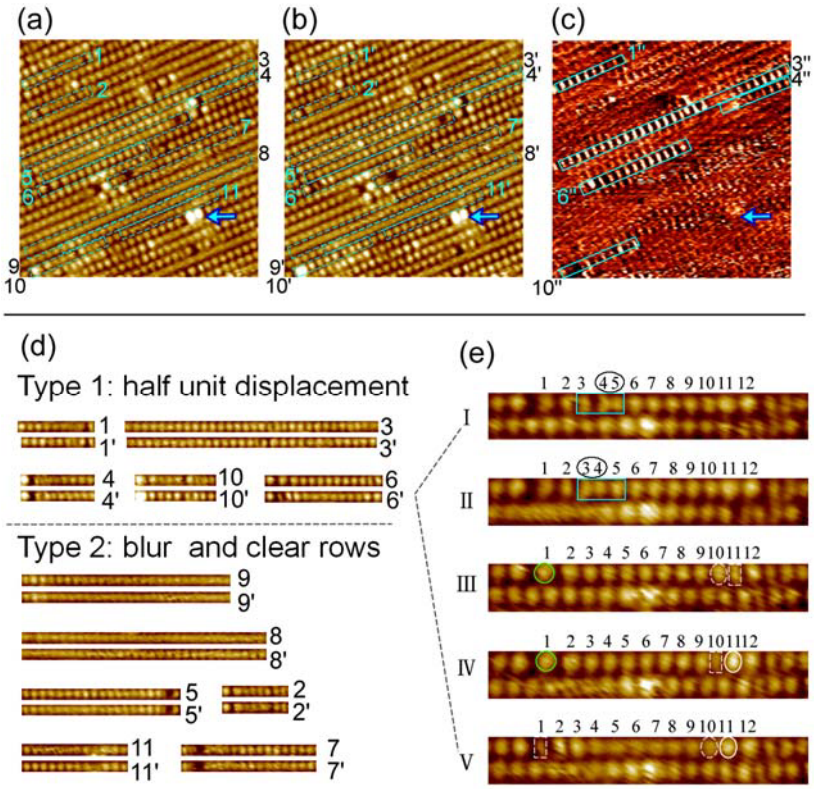

Fig.2 flip-flop phenomenon of Sr/Si(111)- 3x2 surface, (a) and (b) were the same area obtained sequentially within 3 min, (c) was the image obtained by the subtraction of (a) and (b). Scanning condition of V_{bias}=3.0V, I_{set}=20pA, 22×22nm^2 (d) two type changes appearing in (a) and (b). (e) Five sequenced image show the change for line 6.

Fig.3 display a model to explain the Sr atom motion mechanism in this 1D diffusion.

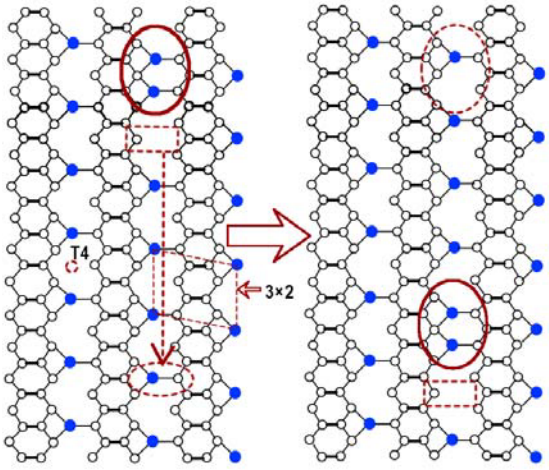

Fig.3 schematic mechanism for Sr atom motion along the channel formed by double bond Si atom

4. Summary

In conclusion, Sr/Si(111)-3x2 surface was investigated by STM. As for the geometric structure, this surface can be described by HCC model with Sr coverage of 1/6 ML. Blur rows appearing in the room temperature STM images arouse from Sr atoms motion phenomenon between two adsorption sites with comparable surface energy, and this show that Sr/Si(111)-3x2 surface behave the quazi-1D property.

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