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Defect-induced Si(100) dimer buckling structures studied by scanning tunneling microscopy

Michihiro Uchikawa [a], Masahiko Ishida [a], Koji Miyake [a], Kenji Hata [a], Ryozo Yoshizaki [b], Hidemi Shigekawa [a,*]

[a] *Institute of Materials Science, and Center for TARA (Tsukuba Advanced Research Alliance), University of Tsukuba, Tsukuba 305, Japan*

[b] *Institute of Applied Physics, Center for TARA (Tsukuba Advanced Research Alliance), and Cryogenics Center, University of Tsukuba, Tsukuba 305, Japan*

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Abstract

The effect of atomic-scale defects on a Si(100) surface dimer buckling structure was studied by scanning tunneling microscopy at about 80 K. The double dimer vacancy (type B) defect was found to induce buckling of adjacent dimers. A similar dimer buckling structure was also observed for single dimer vacancy (type A) defects; however, a kind of type A defects suppressed buckling of adjacent dimers even at low temperature. Phase shift of dimer buckling structure introduced by defects was accounted for by the strain structures in defects.

Keywords: Scanning tunneling microscopy; Silicon; Surface defects; Surface relaxation and reconstruction

1. Introduction

From microscopic analysis by scanning tunneling microscopy (STM), atomic-scale defects in material surfaces have been found to play an important role in the physical and chemical properties of materials. Since differences in the characteristics of defects can be visualized on the Si(100) surface by observing the dimer buckling structures which surround defects, it is intriguing and important to study the defects on the Si(100) surface on an atomic scale. Hamers et al. defined three typical types of defects on the Si(100) surface: type A, single dimer vacancy; type B, double dimer vacancy; and type C, two half-dimers as a result of two missing adjacent Si atoms along the ⟨110⟩ direction (Ref. [1]). Since only type C defects showed a strong metallic character in spectroscopic studies (Ref. [1]), it was considered to form a surface state which causes Fermi level pinning. At room temperature, type A and type B defects did not give rise to any detectable static buckling of adjacent dimers, however, type C defects led to buckling of the adjacent dimers. On the other hand, at low temperature (~140 K), Tochihara et al. showed that the buckling structure of dimers in a region adjacent to the type C defect was found to be symmetric, different from that observed at room temperature (Ref. [2]). Therefore, in order to clarify and understand the characteristic of the other defects, it is necessary to study them at low temper-

* Corresponding author. Fax: +81 298 557440; e-mail: hidemi@mat.ims.tsukuba.ac.jp.

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ature. In this paper, we present the results for Si(100) surface defects obtained by STM at low temperature.

2. Experimental and results

A p-doped (n-type, $\sigma = 0.01\ \Omega\,\mathrm{cm}$) Si(100) sample, oriented to within 0.5° of the (100) direction, was prepared by heat treatment at ~1200°C following an overnight degasing at 450°C. The base pressure was 2×10^{-8} Pa. Tungsten tips were electrochemically etched in NaOH solution and heated in vacuum before use.

STM observation was performed initially at room temperature. Three typical defects, type A, type B, and type C, as defined by Hamers et al., were observed (Ref. [1]). Type A and type B defects do not give rise to any detectable static buckling of adjacent dimers, and type C defects induce buckling of dimers adjacent to the defect. These results agree with the results obtained previously. In addition to these defects, another type of defect which consists of a combination of type A and type B defects with a dimer sandwiched in between was often observed. We call this type U in this paper. Type U defects did not induce buckling of adjacent dimers at room temperature, similarly to type A and type B defects.

In order to clarify the characteristics of the defects, a Si(100) surface was observed by STM at low temperature. Figs. 1a and 2 show STM images obtained at 78 K ($V\mathrm{s} = -1.3$ V, $I\mathrm{t} = 5.0$ nA). As shown in Fig. 1, the single dimer vacancy defect (type A) is further divided into three types (A_1, A_2 and A_3) at low temperature. Type A_1 suppresses buckling of adjacent dimers even at low temperature. Type A_2 induces in-phase buckling on both sides. Type A_3 induces out-of-phase buckling on both sides of the defect. Schematic structures of type A_2 and type A_3 are shown in Figs. 1b and 1c, respectively. As regards the double dimer vacancy defect (type B) indicated by letter B in Fig. 1a, out-of-phase buckling of adjacent dimers was also observed around them, contrary to the result obtained at room temperature.

Type C defects are known to induce a phase shift of the buckled dimers as previously reported (Ref. [2]). In fact, as indicated by letter C in Fig. 1a, a phase shift of the buckled dimers from $c(4 \times 2)$, which is considered to be the most stable phase (Ref. [2]), to $p(2 \times 2)$ is induced. Since such phase shift often occurs in the vicinity of a step edge, defect are thought to have a stronger effect on dimer buckling than the interaction existing between dimer rows even in regions near the step edge. Buckling was clearly observed on both sides of the Type C defect, contrary to the previous result obtained for a type C defect (Ref. [2]). In this case, other defects exists in the neighboring row. According to the results by Tochihara et al., defects do not affect the structure of the neighboring rows (Ref. [2]). But further experiment is necessary. As indicated by C′ in Fig. 2, there exists another type of defect which is similar to type C. The type C′ defect has three half-dimers as a result of three missing adjacent Si atoms along the $\langle 110 \rangle$ direction. As is expected from the characteristics of a type C defect, it does not induce a phase shift into buckled dimers on both sides of the defect.

The type U defect is a combination of type A and type B defects with a dimer sandwiched in between as shown in Fig. 1a by U_1 and U_2 (Ref. [3]). These letters have a similar meaning as A_1 and A_2; U_1 suppresses buckling, and U_2 induces out-of-phase buckling. The middle dimer in the type U defect was observed as two separate symmetric protrusions. Hamers et al. attributed such a structure to Si atoms with adsorbed hydrogen atoms (Ref. [4]). However, all type U defects observed show the separate symmetric structure. This fact suggests that it is a characteristic of this defect. Symmetric dimer structures were often observed around a cluster of type U defects, indicated by the letter Uc in Fig. 1a.

Fig. 3 is a schematic structure of the step edge (Ref. [5]). Solid circles indicate the upper atoms in all dimers. As Hamers et al. pointed out, at the A step, dimers on the upper step edge are strongly buckled (Ref. [4]). And Si atoms on the dimer rows in the lower terrace always move towards the upper direction as shown in Fig. 3. As indicated by arrows in Fig. 3, strain structures seem to play an important role in inducing dimer buckling. Since buckling structure at the step edge is fixed as described above, an additional single dimer row

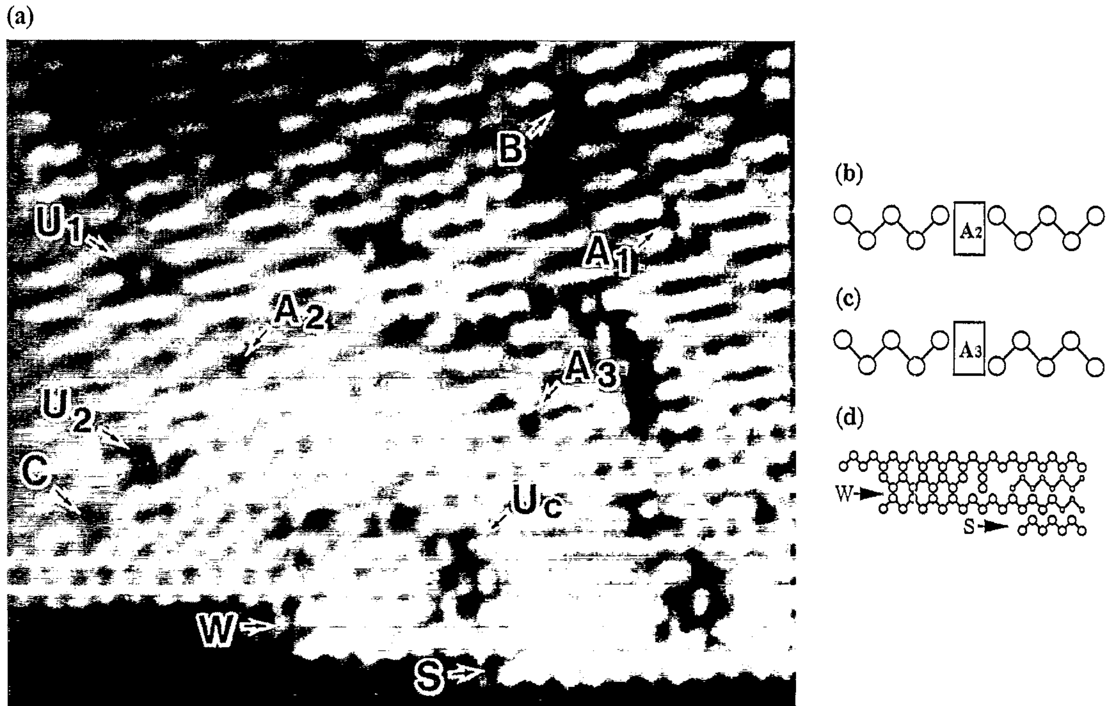

Fig. 1. (a) STM image of Si(001) obtained at 78 K ($Vs = 1.3$ V, $It = 5.0$ nA). Schematic structures of (b) type A_2 defects, (c) type A_3 defects and (d) step edge.

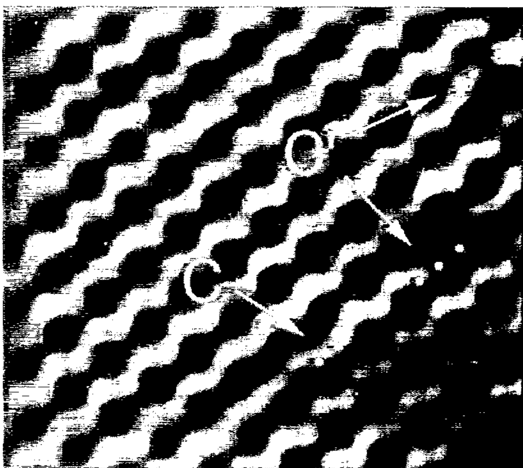

Fig. 2. STM image of Si(001) obtained at 78 K ($Vs = -1.3$ V, $It = 5.0$ nA).

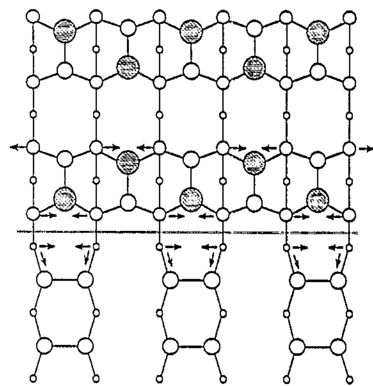

Fig. 3. Schematic model for the dimer buckling structure at A step.

produces a phase shift of the buckled dimers, as indicated by S and W in Figs. 1a and 1d, which means that interaction between adjacent dimer rows is insufficient to change the $p(2 \times 2)$ phase to a $c(4 \times 2)$ phase even near the step edge; the energy difference between those two phases is small.

As shown in Fig. 1, both in-phase and out-of-phase buckling structures are induced by the type A defects. In order to explain the buckling phenomenon, schematic structures of the vacancy defect (V) and the depression defect (D) models are shown

in Fig. 4 (Ref. [6]). If we concentrate on the strain structures of those defects, buckling structures induced by those defects are out-of-phase and in-phase for V and D models, respectively, as shown in Fig. 4. By combining those defects, phase shifts induced by type B defects can also be explained as shown in Fig. 5 (Ref. [7]). If a dimer is sandwiched by two defects, and the strain of the defects tend to move the Si atoms in the dimer toward the same direction, the dimer may be symmetrically stabilized as the Si dimer in the type U defect.

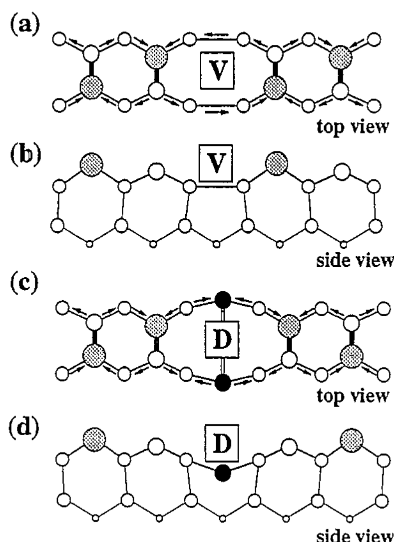

Fig. 4. Schematic structures of the vacancy defect ((a), (b)) and the depression defect ((c), (d)) models.

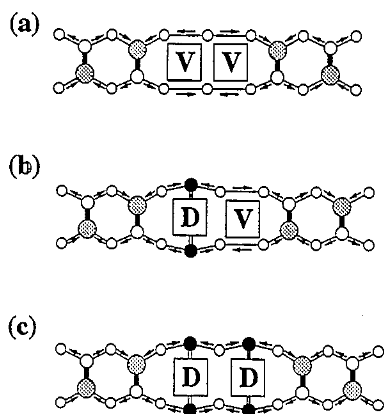

Fig. 5. Structural models for phase shift of buckling dimers.

3. Conclusions

From STM observation of the Si(100) surface at about 80 K, the single dimer vacancy defect (type A) was found to be of three types (A_1, A_2, and A_3) at low temperature: A_1 suppresses buckling of adjacent dimers even at low temperature; A_2 induces in-phase buckling; and A_3 induces out-of-phase buckling. For the double dimer vacancy defect (type B), out-of-phase buckling of adjacent dimers was also observed, contrary to the result obtained at room temperature. As regards the type U defect, which is a combination of type A and type B defects, a Si dimer existing between them was observed as two separate protrusions. We explained the phase shifts of the buckling dimers induced by defects in terms of the vacancy defect and the depression defect models.

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[7] Other structural models are proposed for the defects such as those in Ref. [3]. Similar analysis used here can be applied to those structures. The type B defect model represented by Fig. 4a in Ref. [3] produces the in-phase buckling, which is inconsistent with the observed results. For a type A defect, the model of Fig. 3b in Ref. [3] introduces the out-of-phase buckling. Therefore, other structures are necessary to explain the observed results, which include the defects inducing in-phase and non buckling structures.