Characteristic structures of the Si(111)-7×7 surface step studied by scanning tunneling microscopy

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Contrary to previous results concluding that all 7×7 boundaries in the down step edge were complete, 5×5 faulted half units were found to be introduced in part when the transition region was narrow. In addition, the formation characteristic of the 5×5 faulted half units was strongly influenced by the type of step configuration (nF or nU) and by the structure of the upper step edge (complete or incomplete). Even when the step configuration was the same, the difference in the upper step edge structures strongly affected introduction of 5×5 units. © *2001 American Vacuum Society.* [DOI: 10.1116/1.1359538]

I. INTRODUCTION

The Si(111)-7×7 structure has been extensively studied and the dimer-adatom-stacking (DAS) fault model is widely accepted to explain the structure.[1-3] However, since it has a complicated structure, the study of its stability and phase transition mechanism is still one of the most important targets of recent researchers.[4-10] Since nucleation and growth of the 7×7 phase is governed at the step,[11-14] analysis of the step structures gives information about the stability of DAS structures upon phase transition. In addition, analysis of atomic structures of steps on the surfaces is important both scientifically and technologically because they play an important role in, for example, chemical reactions and crystal growth by molecular beam epitaxy. From this point of view, atomic structures of the steps on the Si(111)-7×7 surface have been studied by using scanning tunneling microscopy (STM).

Becker *et al.* reported the first STM image of the steps on Si(111)7×7. They observed only one type of step structure, namely, both the upper and lower terrace edges were perfectly matched at a step by forming 7×7 units.[15] However, as Tochihara *et al.* pointed out, taking into consideration the phase mismatching between the DAS structures formed on upper and lower terraces at a step edge, 14 different type structures are possible. First, there exist two possibilities: whether the upper terrace is terminated by the edge of the faulted half or of the unfaulted half triangles as shown in Fig. 1.[16] They were named the F step and the U step, respectively. Then, seven different step types are possible for each F and U step, as determined by the distance L (Fig. 1) between the 7×7 phase boundary on the lower terrace and the step. The distance L can be represented as $[(3n+4)/21]a$ for the F step and $[(3n+2)/21]a$ for the U step. Here, n is an integer between 0 and 6 and a is the length of the 7×7 half unit triangle (Fig. 1). According to the value of n, steps are called nF or nU steps. For a value of n from 1 to 6, a region the size of which is shorter than the length of the 7×7 half unit, a, is introduced. The area is called the transition region.

Several years ago Wang and Tsong performed a systematic study of the structures of atomic steps of the Si(111)-7×7 surface,[17] and they observed all of the 14 different type steps described above. According to their results, in most cases, the effect of phase mismatching at the step was limited in the transition region. That is, U and F steps were terminated by complete 7×7 units, and the boundary of the 7×7 phase on the lower terrace was also complete. The transition region was a disorder phase and a smaller DAS structure such as a 5×5 one did not appear even though there was enough space for the formation of the structure such as $5U$ and $6U$ steps. In some cases, $0U$, $1U$, $4F$, and $5F$ upper step edges did not coincide with the complete 7×7 unit boundary. However, the boundary of the 7×7 phase on the lower terrace was complete even in the cases.

As is known well, the presence of a step reduces the surface symmetry and increases the number of dangling bonds. The local structures around a step are determined by the competition between the increase in the strain energy and the reduction of the number of dangling bonds, similar to surface reconstruction. Therefore, in spite of the results of Wang and Tsong,[17] various kinds of structures are expected to be formed around steps, such as the introduction of faulted halves of smaller size. In fact, Tochihara *et al.* reported that 5×5 faulted half units were formed on the lower terrace in the case of $5U$ steps.[16] A similar structure, the introduction of 5×5 units, was observed in the phase boundaries on the terrace to stabilize the structure.[18]

In this article, from the standpoint described above, we reexamined the structure of Si(111)-7×7 steps. For a wide

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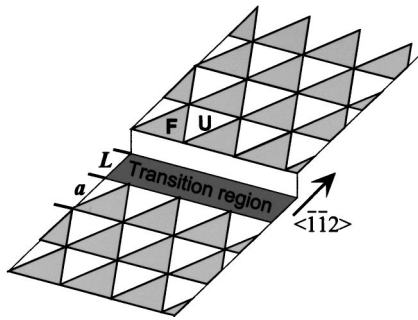
FIG. 1. Illustration of a step structure. *F* and *U* represent the faulted and unfaulted half units of a 7×7 structure, *a*: Length of the 7×7 half unit triangle; *L*: width of the transition region.

transition region, there was no faulted half unit of any size within the regions, which agrees well with the results of Wang and Tsong.[17] However, we found that 5×5 faulted half units were partly formed in 7×7 faulted half units in the boundary on the lower terrace when the transition region was narrow.

II. EXPERIMENTS

Phosphorus-doped *n*-type Si(111)(ρ=0.375–0.625 Ω cm) substrates were used in this study. The samples were chemically cleaned by acetone before being loaded into the ultra-high vacuum (UHV) chamber. The samples were outgassed at ~500 °C for 12 h. Subsequently, the samples were flashed at about 1250 °C for 15 s in order to form the 7×7 structure following slow cooling. The base pressure was less than 8 $\times 10^{-9}$ Pa and the pressure during the flashing process was kept below 2×10^{-8} Pa. All STM observations were performed at room temperature using an electrochemically etched tungsten tip and all STM images shown here were obtained in the constant current mode.

III. RESULTS AND DISCUSSION

Figure 2 shows STM images of 1*F* and 2*U* step edges of a Si(111)-7×7DAS structure. The sample bias voltages are +0.5 V (empty state) for Figs. 2(a) and 2(c) and −0.5 V (filled state) for Figs. 2(b) and 2(d). The steps observed are straight, and the upper terraces of the steps are terminated by the almost complete boundaries of the 7×7 unit cells at the step edge (complete step edge).

Next, let us focus on the structure of the down steps. In the case of the 1*F* step, 7×7 unfaulted half units form the straight boundary shown in Figs. 2(a) and 2(b). There is a transition region between the 7×7 boundary and the step edge. We cannot find peculiar results differing from the structures observed in previous work.

On the other hand, a peculiar structure, which has a characteristic adatom arrangement differing from the normal 7 ×7 adatom arrangement, was found in the case of the 2*U* step, and it is shown by triangles in Figs. 2(c) and 2(d). Figures 3(a) and 3(b) show a magnified STM image of the observed characteristic structure of the empty state and the filled-state, respectively. The *N* and *C* in Fig. 3 represent the
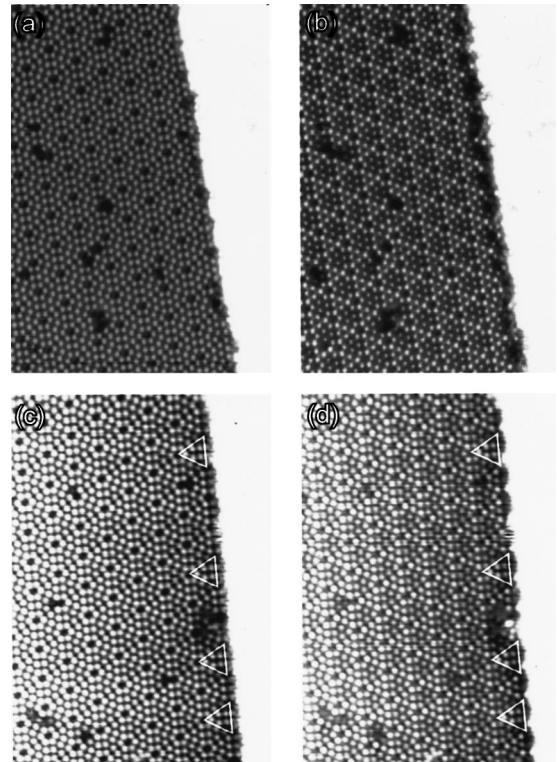

FIG. 2. STM images of (a), (b) 1*F* and (c), (d) 2*U* steps. The sample bias voltages are +0.5 V for (a) and (c) and −0.5 V for (b) and (d). Setting tunneling current is 0.3 nA. The triangles in (c) and (d) indicate the characteristic structure. The upper step is out of contrast.

normal and the characteristic half units, respectively. The arrows in the filled state STM image [Fig. 3(b)] indicate that the adatoms observed were darker than those in the normal 7×7 arrangement. The brightness of the adatoms in the 7 ×7DAS structure in the filled-state STM image reflects their second and third layer structures, i.e., the number of rest atoms around the adatoms.[8,18,19] Therefore, the adatoms indicated by arrows in Fig. 3(b) are surrounded by more rest atoms than normal 7×7 adatoms. On the basis of this, we
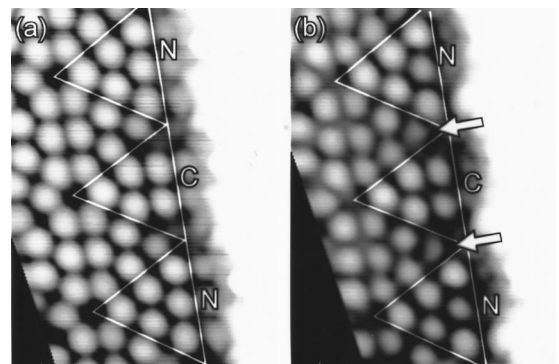

FIG. 3. Magnified STM images of the characteristic structure in Fig. 2. The sample bias voltage and setting current are (a) +0.5 V and 0.3 nA and (b) −0.5 V and 0.3 nA. *N* and *C* represent the normal and the characteristic half units, respectively. The arrows indicate the adatoms that were observed to be darker than those in the normal 7×7 arrangement. The upper step is out of contrast.
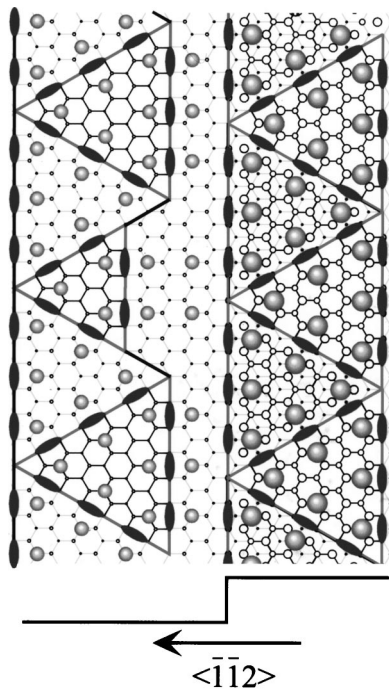
FIG. 4. Schematic model of the characteristic structure in Fig. 3.

can conclude that the characteristic structures observed consist of 5×5 faulted half units, as shown in Fig. 4 schematically. Therefore, the 5×5 structure is introduced in the step region as expected.

Next, we consider the correlation between the conformation of the upper step edge and the emergence of the characteristic structure. Figure 5(a) shows an empty state STM image of a step structure. Here, straight and zigzag structures coexist at the step edge. There are two phase boundaries, indicated by arrows in Fig. 5(a), and magnifications of them
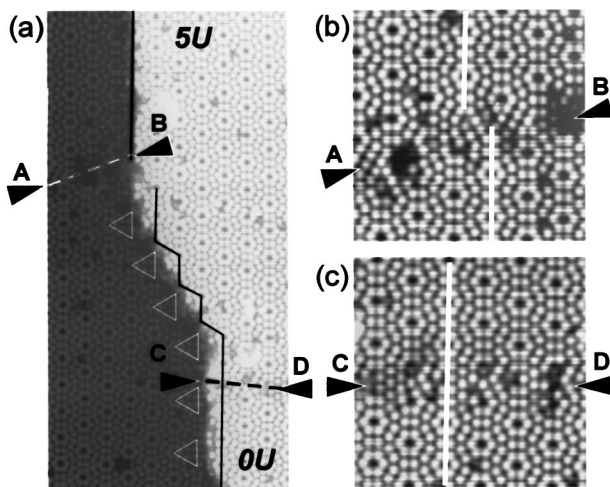

FIG. 5. (a) An empty state STM image of a step structure. Two phase boundaries are indicated by arrows in the image. White triangles show the 5×5 faulted half units introduced. The dashed lines indicate the phase boundaries. (b), (c) Magnified STM images of phase boundaries $A-B$ and $C-D$ in (a). In (b) and (c), the vertical lines through the phase boundaries show the phase shift between two 7×7 domains.

are shown in Figs. 5(b) and 5(c). Phase mismatching at the boundary $C-D$ is in the direction of $[\bar{1}10]$, which does not influence the step configuration between lower and upper steps. On the other hand, the phase boundary $A-B$ has an influence on the step configuration because the phase mismatch is in both directions, $[\bar{1}10]$ and $[11\bar{2}]$. As a result, the step types changed across the phase boundary, namely, from $5U$ on the upper side to $0U$ on the lower side.

It is clear that the structure of the upper step edge changes due to the change in step type. At the $5U$ step, the upper step edge coincides with the complete 7×7 unit boundary similar to in the previous results.[16,17] On the other hand, at the $0U$ step, there are two types of structure of step edge. One is the upper edge which consists of the 5×5 unfaulted half unit separated by open 7×7 faulted subunits (incomplete $0U$ step), which is the same structure as that obtained by Wang and Tsong.[17] The other is the structure where the upper step is terminated by the complete 7×7 unfaulted unit cell (complete $0U$ step), corresponding to the STM image obtained by Becker *et al.*,[15] that is, the structure of the upper step edge changes even when the type of step configuration is the same. Therefore, the structure of the lower step edge also changes, possibly depending upon the structure of the upper step edge. Let us discuss this point next.

In the case of the $5U$ step, the boundary of the 7×7 phase on the lower terrace is complete. The transition region is a disorder phase and any smaller size DAS such as the 5×5 structure did not appear even though there was enough space for formation of the structure. This result agrees with the result of Wang and Tsong.[17] However, in the case of the $0U$ step, a new structure appeared on the lower terrace. The 5×5 faulted half units, which are represented by triangles in Fig. 5, were introduced between the complete 7×7 faulted half units along the step. The 5×5 faulted half units were frequently observed especially when the upper edge has the same structure as that observed by Wang and Tsong: a 5×5 unfaulted half unit separated by open 7×7 faulted subunits. This tendency is clearly seen in Fig. 6. In Fig. 6, a phase boundary exists on the upper terrace, and the step types across the phase boundary have changed from $0U$ on the upper side to $3U$ on the lower side. At the complete $0U$ step along the dotted lines, there was a wide transition region instead of the appearance of any size of the faulted half units, even when the transition region was wide enough to form 5×5 and/or 7×7 faulted half units. On the other hand, 5×5 faulted half units were frequently observed on the lower terrace at the incomplete $0U$ step, with the 5×5 structure indicated by the triangles.

It is noted that 5×5 faulted half units are introduced only when the transition region is narrow, such as in the case of $0U-2U$ steps. They were not observed in the wide transition region such as in the case of $3U-6U$ steps as shown in Figs. 5 and 6. These facts indicate that the width of the transition regions primarily affects the introduction of 5×5 faulted half units. Then, the introduction of 5×5 faulted structures may reduce the strain energy further depending upon the structure of the upper step edge.
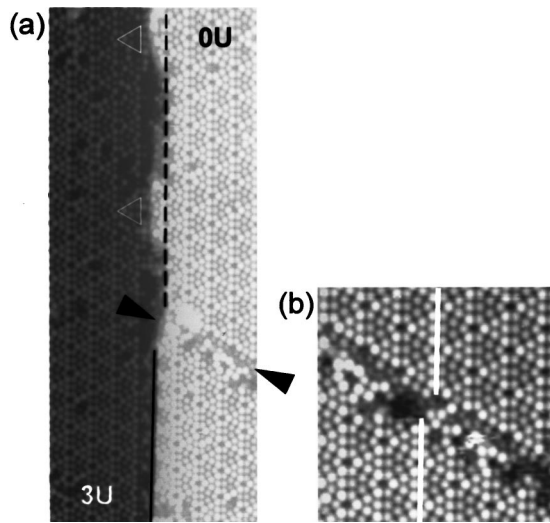
FIG. 6. (a) Filled state STM image of a step structure. A phase boundary is indicated by arrows. (b) Magnified STM image of the phase boundary in (a). The vertical lines through the phase boundary show the phase shift between two 7×7 domains.

When the transition regions are wide, the strain will be relaxed in the transition region. As a result, it has no use for further formation of 5×5 faulted half units. On the other hand, when the transition region is narrow, the structure of the step affects the stability of the dimers existing along the step edge on the lower terrace. If dimers are formed on both the upper and lower step edges as in the case of the complete $0U$ step, the configuration of the densely formed dimers is considered to be unstable. As a result, dimers on the lower terrace become broken and a wider transition region is formed instead. Furthermore, when the upper edge of the $0U$ step consists of the 5×5 related structure (incomplete $0U$ step), the structure makes the transition region narrower compared to the complete $0U$ step. Namely, the width of the transition region becomes virtually equal to that of the $2U$ step. Then, the 5×5 faulted half units may possibly be introduced on the lower edge of the incomplete $0U$ step. It is remarkable that the 5×5 faulted half units are not formed
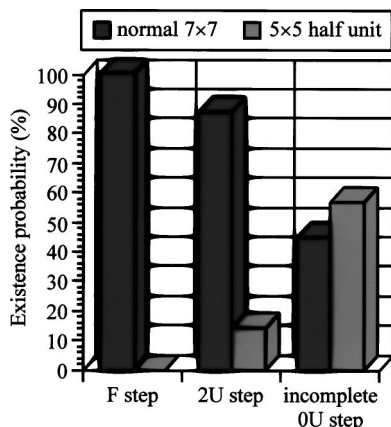

FIG. 7. Existence probability of 5×5 faulted half units at the lower step edge counted from the STM images.

joined to each other, namely, there exists a certain space between the 5×5 structures, as clearly seen in Fig. 5. An optimum structure must exit.

Finally, the existence probability of 5×5 faulted half units is considered to be different from each other because the structure of an upper step edge is different. Figure 7 shows an example of the existence probability of 5×5 faulted half units at the lower step edge counted from the STM images. No characteristic structure was observed at the lower F step edge. On the other hand, in the case of the U step, the existence probability at $2U$ and incomplete $0U$ steps are 0.13 and 0.56, respectively. These results clearly indicate as expected that the introduction of 5×5 faulted half units is affected by not only the width of the transition region but also by the structure of the upper step edge.

IV. CONCLUSION

We found for the first time that the formation of 5×5 faulted half units strongly depends on both the width of the transition region and the structural integrity of the upper step edge. This result indicates that the structures of the upper and the lower step edges are determined by the energetic competition between the formation of transition regions and the structural integrity of the upper step edge as expected.

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