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Pseudo-Real Time Observation of the Dynamics of Phase Defect on Si(100) Surface

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The dynamics of a phase defect (P-defect) on the Si(100) surface was studied for the first time by scanning tunneling microscopy in pseudo-real time below 10K, using the repeated-line-scan technique in which single line scans are repeated on the same path along a dimer row. In addition to the pair creation and annihilation of the P-defect, the effect of a step on the motion of the P-defect was clearly demonstrated. Since the local barrier height for the migration of the P-defect depends on the local environment such as strain and electronic structure due to the existence of defects or dopants, the obtained results also indicate that analysis of the P-defect is promising for local probing of the Si(100) surface. [DOI: 10.1143/JJAP.41.5017]

KEYWORDS: scanning tunneling microscopy, Si(100), defect, low temperature, phase transition, dimer, step

1. Introduction

Top-layer Si atoms of the Si(100) surface form dimers in order to reduce the surface energy, resulting in a (2×1) structure.[1)] In fact, the first scanning tunneling microscopy (STM) observation at room temperature showed a symmetric dimer (2×1) structure.[2)] However, as is now well known, dimers buckle for further energy reduction, and the observed symmetric dimers are considered to represent an averaged view of the thermally activated flip-flop motion of the buckled dimers. Along a dimer row, dimers alternately buckled in opposite orientations. Therefore, two configurations are possible for the buckled dimer arrangement: one is the $c(4 \times 2)$ phase which has antiphase arrangement between two adjacent dimer rows, and the other is the $p(2 \times 2)$ phase which has in-phase arrangement. Many theoretical calculations indicate that the $c(4 \times 2)$ phase is the more stable structure.[1)] At low temperature (140 K ∼ 80 K), the buckled dimer $c(4 \times 2)$ phase was observed, by STM[3)] and low energy electron diffraction (LEED),[4)] to cover the surface. Therefore, $c(4 \times 2)$ was concluded to be the ground state of this surface and was considered to remain stable at lower temperature. However, recently, $p(2 \times 2)/c(4 \times 2)$ mixed,[5)] anomalous flip-flop (apparent symmetric dimer),[6)] and symmetric dimer (no flip-flop motion)[7)] phases were observed by STM below 20 K, and the $c(4 \times 2)$ phase was not observed. These results again give rise to much contradiction concerning this issue. Very recently, more detailed STM investigation clarified the following:[8)] (1) the stable structure below 10 K depends on the type of dopant; the $c(4 \times 2)$ phase remains only for the p-type substrate, and the $p(2 \times 2)$ single phase appears for the n-type substrate, (2) mixture of the $c(4 \times 2)$ and $p(2 \times 2)$ phases and the fluctuation between them is induced by the introduction and dynamics of the P-defect (a phase defect), (3) symmetric dimer phases caused by bias dependence and STM tip-induced flip-flop motion appear at low temperature. However, even considering all these results, the low-temperature issue still remains an enigmatic subject concerning the Si(100) surface. The P-defect is a phase defect with a structure similar to that of the C-defect; it consists of two adjacent dimers which buckle with the same orientation.[5)] However, the P-defect can migrate along a dimer row, unlike the C-defect, as one of its two dimers changes orientation (Fig. 1). If a P-defect exists on a dimer row, it serves as a phase shifter and induces phase mixing between $c(4 \times 2)$ and $p(2 \times 2)$. At 80 K, the P-defect tends to migrate to reduce the $p(2 \times 2)$ area because $c(4 \times 2)$ is more stable than $p(2 \times 2)$ at this temperature.[9)] On the other hand, at 5K, fluctuation among $c(4 \times 2)$ and $p(2 \times 2)$ phases is due to the weak interactive migration of P-defects.[5)] Therefore, an understanding of the dynamics of P-defect is important in determining the stability of the surface phase. As a result of a recent increase in the attention paid to nanoscale science and technology, the Si(100) surface is expected to be used as a template, in combination with organic materials, to develop new functional devices. However, it is well known that surface local structures such as defects, steps and dopants influence the local electronic and geometric structures of the Si(100) surface.[11,12)] From this point of view, it is extremely important to investigate the effect of such local structures. Since migration of the P-defect is induced by the flip-flop motion of the dimers which reflects the local barrier height,[13)] and the barrier height depends, for example, on the local strain and electronic structures due to the existence of defects and dopants, the P-defect is promising as a probe of the external field introduced by the local environment. For the reasons described above, real-time analysis of the P-defect is extremely important and useful. However, until now, detailed dynamics of the P-defect could not be determined, because the conventional scanning method requires at least several ten seconds to obtain one image, and it is too slow to follow the dynamics of the P-defect. In this study, we investigated the dynamics of the P-defect by the repeated-line-scan technique in which single line scans are repeated on the same path along a dimer row.[14)] By this method, (1) the creation and annihilation of the P-defect, and (2) the influence of a step on the motion of the P-defect were clearly observed in real time.

2. Experimental

An As-doped (∼ 0.003 Ω·cm) Si(100) sample was cleaned by heating to ∼ 1200°C after prebaking for one day; the pressure during the heat treatment was kept below 5×10^{-8} Pa. Measurements were performed at 10 K in ultrahigh vacuum (5×10^{-9} Pa) using a W tip. Sample temperature was moni-

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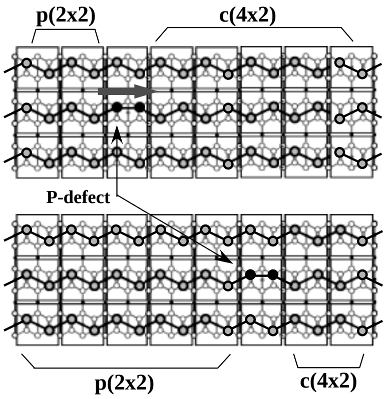

Fig. 1. Schematics of the P-defect and its movement caused by dimer flip-flop motion.

tored with a thermocouple.

3. Results and Discussion

3.1 Method of analysis of the P-defect dynamics

Figure 2 shows a typical STM image of the Si(100) surface obtained below 10 K. When defect density is low, the p(2 × 2) phase is dominant on this surface.[8)] There exist some P-defects at the boundaries between c(4 × 2) and p(2 × 2) phases as indicated by arrows. Figure 3(a) show an STM image of a P-defect. In the STM image, there exists a dark region in the dimer row indicated by an arrow. Under these conditions (sample bias: 0.6 V, tunneling current: 0.2 nA), P-defects appear darker than normal dimers. As can be seen in Fig. 3(a), the dimer arrangements on the left and right sides of the dark region are c(4 × 2) and p(2 × 2) phases, respectively. And this region migrates along the dimmer row. Therefore, the noisy dark region is a movable phase shifter and corresponds to the position of the P-defect. Figure 3(b) is the time-versus-position pseudoimage obtained along the single dimer line with the P-defect indicated by an arrow in Fig. 3(a). Here, the same single dimer row was scanned repeatedly; the time evolution of the change is shown on the longitudinal axis. The image consists of 800 lines, and each line was scanned at the rate of 0.25 s/line. Since dimers are alternately buckled in opposite orientations, the periodicity of $2a_0$ ($a_0 = 0.38$ nm, surface lattice constant) is shown along the dimer row in Fig. 3(b). Figure 4 shows the schematic of the observed time-versus-position pseudoimage in Fig. 3(b). The grid lines in Fig. 4 indicate the periodicity of the surface lattice constant a_0. Solid circles in Fig. 4 shows the discrete positions of the P-defect determined from the cross sections of the original STM image in Fig. 3(b). This image clearly shows that migration of the P-defect is caused by the jumping of the P-defect in the step of the surface lattice constant. By plotting a histogram of this discrete graph, we can analyze the effect of the local environment on the dynamics of

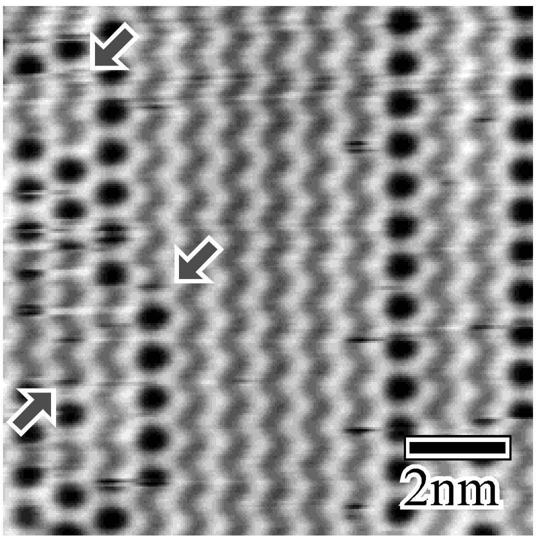

Fig. 2. A typical STM image of Si(100) surface obtained below 10 K (sample bias: 0.8 V, tunneling current: 1.0 nA). Some P-defects are indicated by arrows.

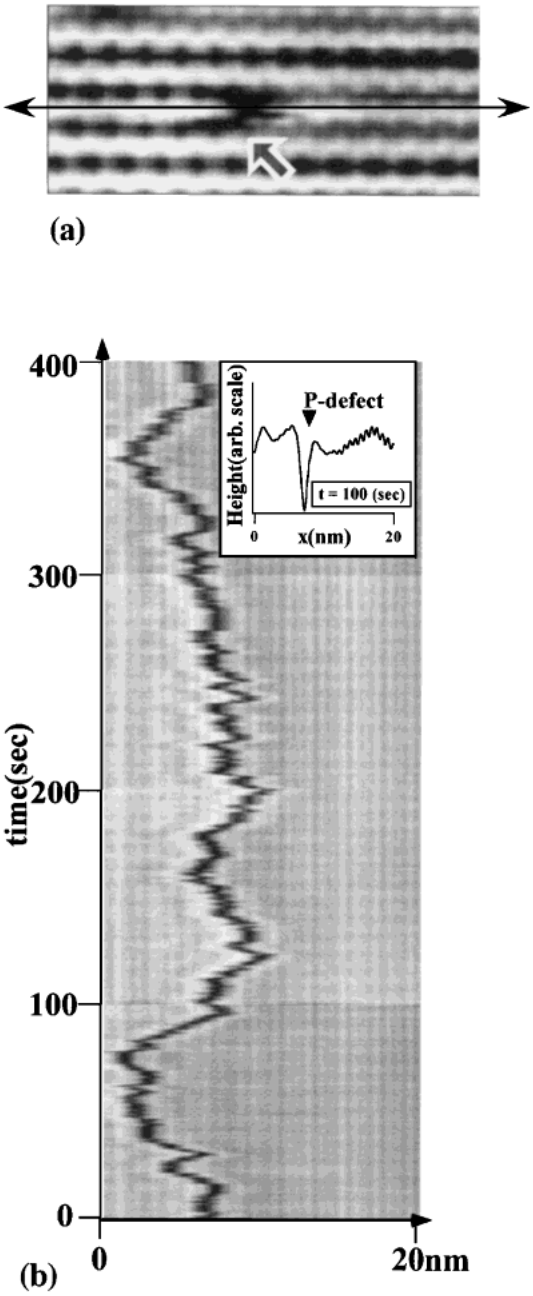

Fig. 3. (a) STM imge of a P-defect (sample bias: 0.6 V, tunneling current: 0.2 nA). (b) Time-versus-position pseudoimage obtained along the dimer row with a P-defect indicated by an arrow in (a).

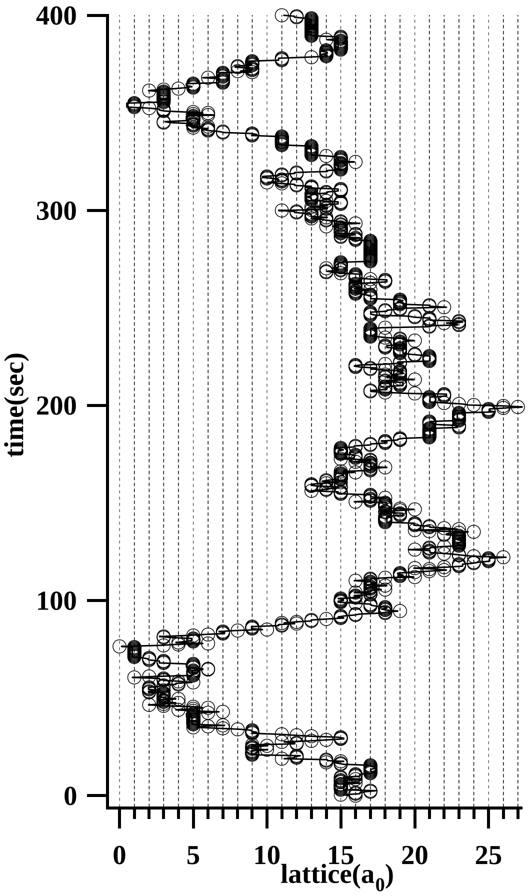

Fig. 4. Schematic of the observed time-versus-position pseudoimage in Fig. 3(b). The grid lines indicate the periodicity of a_0 ($a_0 = 0.38$ nm, surface lattice constant). Solid circles shows the discrete positions of the P-defect determined from the cross sections of the STM image in Fig. 3(b).

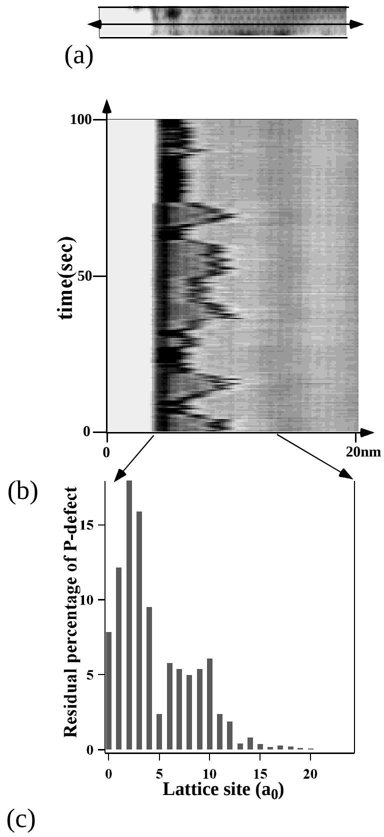

Fig. 5. (a) STM image of a P-defect near a step edge. (b) Time-versus-position pseudoimage of the P-defect along the dimer row indicated by an arrow in (a). (c) Histogram presenting the residence percentage of the P-defect shown in (b).

the P-defect.

3.2 Effect of a step on the dynamics of P-defect

It has been suggested that steps and defects have greatly influence the dimer structures of the Si(100) surface.[11] In order to apply our technique to investigating this issue, we observed the dynamics of a P-defect near a step edge. Figure 5(b) shows a time-versus-position pseudoimage of the P-defect near a step shown in Fig. 5(a). There is a step on the left side in the scan area, which is imaged white since contrast is adjusted to the lower terrace. As clearly shown in Fig. 5(b), the P-defect migrates in the narrow region near the step edge on the left side. In order to examine the characteristic property of the P-defect in greater detail, a histogram representing the residence percentage of the P-defect along the dimer row is shown in Fig. 5(c), as obtained by a method similar to that for Fig. 4. It is clear that there exists a strong influence of the step edge on the migration of the P-defect. As mentioned in §1, since the dynamics of the P-defect reflects the local barrier height which governs the buckling of the dimer in the P-defect, the P-defect is promising as a local probe which is sensitive to the external field introduced by the local environment. In this case, an attractive interaction exists near the step edge. The existence of a local effect is clear. However, since the dynamics of the P-defect is influenced by many other factors, such as the surrounding phase structure, other defects, and the tip effect, further analysis is necessary for understanding the observed effect in detail. Such analysis is now in progress.

3.3 Pair creation and annihilation of P-defects

When the surface is covered by a single phase, p(2 × 2) or c(4 × 2), P-defects are considered to be introduced through the thermal activation of the dimer flip-flop motion.[15–17] Since the P-defect is a phase shifter, its existence induces the mixing of the c(4 × 2) and p(2 × 2) phases, resulting in an increase in the surface energy. Flip-flop of the only one dimer is enough to create a P-defect from other defects or steps. However, on the terraces, since P-defects act as phase shifters, they must be created in the form of a pair, as shown in Fig. 6. Therefore, at low temperature, they are considered to be generated mainly from other defects and steps, i.e., through low-energy paths.[9] However, when some perturbation with sufficient energy is applied to the surface, P-defects are expected to be created. Figure 7 shows a time-versus-position pseudoimage of the Si(100) surface. At point A, a pulse bias (0 V to 5 V) was applied from the STM tip during the scan. It is clear that four (two pairs of) P-defects were created by the pulse bias. Migration of the P-defects was subsequently observed, and pair annihilation occurred at point B. This is the first direct observation of the creation and annihilation of the P-defect in pseudo-real time. P-defects can be introduced as a local probe by using the above technique, making it possible to analyze their dynamics even in a single-phase surface area.

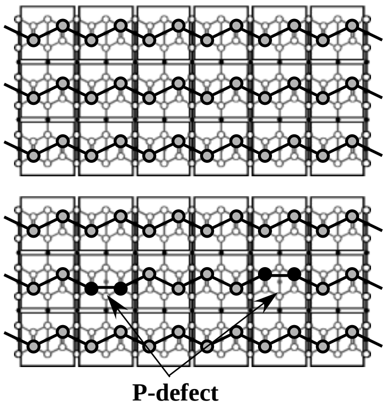

Fig. 6. Schematic of the creation of a pair of P-defect.

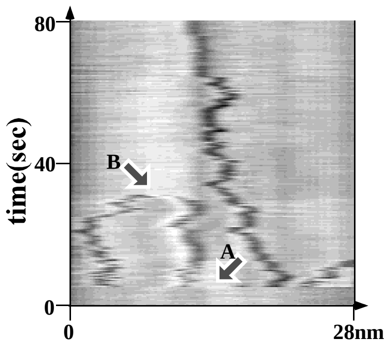

Fig. 7. Time-versus-position pseudoimage of the creation and anhilation of P-defects.

4. Conclusion

Dynamics of the P-defect on a Si(100) surface was studied for the first time by STM in real time below 10 K, using the repeated-line-scan technique. In addition to pair creation and annihilation of the P-defect, the effect of a step on the motion of the P-defect was clearly demonstrated. Since the local barrier height for the migration of the P-defect depends on the local environment such as strain and electronic structure due to the existence of defects or dopants, the obtained results also indicate that analysis of the P-defect is promising for local probing of the Si(100) surface.

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