Single-domain Si(110)-16×2 surface fabricated by electromigration

Yoichi Yamada, Antoine Girard, Hidehito Asaoka, Hiroyuki Yamamoto, and Shin-ichi Shamoto
Quantum Beam Science Directorate, Japan Atomic Energy Agency, Tokai, Naka, Ibaraki 319-1195, Japan
(Received 22 May 2007; published 23 October 2007)

Micrometer-wide single domain of Si(110)-16×2 reconstruction has been fabricated by means of controlled electromigration of surface atoms. The electromigration effect in dc heating process is found to line up the reconstruction rows when the current direction matches the orientation of the rows. This finding provides not only a well-controlled surface preparation method for Si(110) but also another template for low-dimensional nanostructures.

DOI: 10.1103/PhysRevB.76.153309 PACS number(s): 68.47.Fg, 68.35.Bs, 68.55.Jk, 68.37.Ef

Si(110) surface is currently attracting renewed interests because of its unique properties such as high hole mobility,[1,2] peculiar surface reactivity,[3] and strong morphological anisotropy.[4] Si(110) surface is going to be used in the vertical ("fin-type") double-gate metal-oxide-semiconductor field effect transistor devices that enable much more high integration.[5] The strong structural anisotropy of surface has been utilized to grow one-dimensional nanostructures on the surface.[4] Despite these increasing requirements, the number of studies on Si(110) has been small, and many basic properties including surface atomic structure remain unsolved. This situation is quite different from the cases of other low-index surfaces of Si, (111) and (100), to which tremendous number of works have been devoted. The delay of the studies on Si(110) surface is largely owed to a difficulty in the surface preparation. The clean Si(110) surface exhibits a complicated surface reconstruction called 16×2 with huge unit cell containing a monatomic step,[6] as shown in Fig. 1. Although many structural models[7] (including a recent one based on detailed density-functional theory calculation[6]) have been proposed so far, the surface atomic structure of the 16×2 reconstruction seems to be still unsettled. Scanning tunneling microscopy (STM) studies have revealed that the Si(110) surface is not only complicated but also inhomogeneous. The 16×2 reconstruction typically shows a double-domain structure identified with fragmented rows running along two directions, $[1\bar{1}2]$ and $[\bar{1}12]$, as shown in Fig. 1(a). In addition, disordered structures always coexist randomly.[7] Furthermore, various surface reconstructions other than 16×2 have been found due to small amounts of impurities,[8] suggesting the instability of the 16×2 reconstruction. The inhomogeneity and instability of the surface reconstruction have hindered a detailed understanding of the basic properties of Si(110) such as the surface electronic structure and the surface chemical reaction, as well as the structural determination. Recently, precise angle-resolved photoemission measurement has been conducted using the single domain of Si(110)-16×2,[9] which determined the band dispersion of the surface state along major symmetrical directions. Nevertheless, little attention has been given to the preparation of the single-domain surface so far. For further development of the understanding of Si(110), it is quite important to establish the preparation method for the well-defined single-domain surface of Si(110).

One strategy to realize the well-defined surface of Si(110) would be making use of its instability. Because of the instability, the surface structure of Si(110) can easily be manipulated by a small external perturbation. The perturbation we

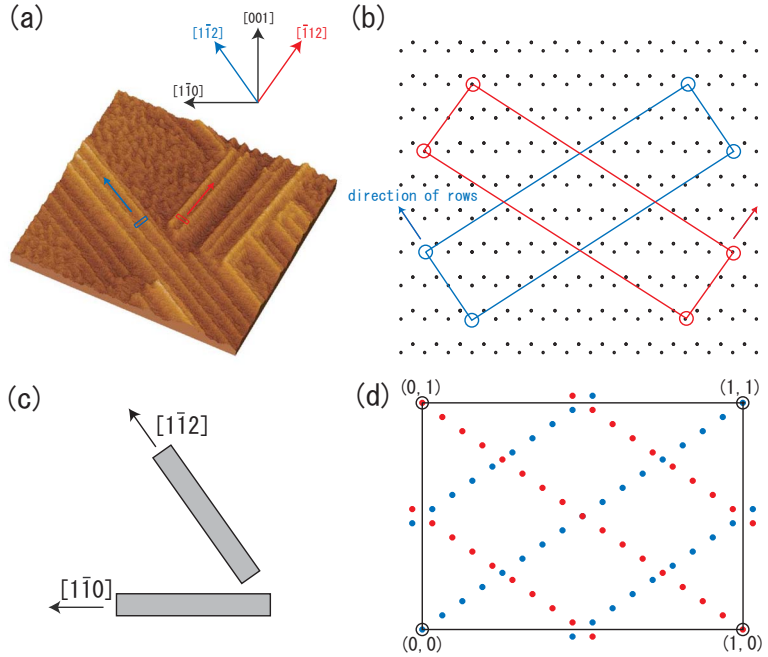

FIG. 1. (Color online) (a) 100×100 nm^2 STM image of typical Si(110)-16×2 reconstructed surface. The reconstruction rows running along $[1\bar{1}2]$ and $[\bar{1}12]$ are indicated by blue and red arrows. Unit cell of 16×2 is schematically shown by red and blue rectangles. Coexisting disordered area can be seen at the top corner. (b) Two equivalent unit cells for 16×2 reconstruction (red and blue). Black dots represent atoms of unreconstructed (110) surface. (c) Schematic drawing of two specimens used in this study. (d) Reciprocal lattice scheme for 16×2 (blue and red dots). Black open circles represent 1×1 spots.

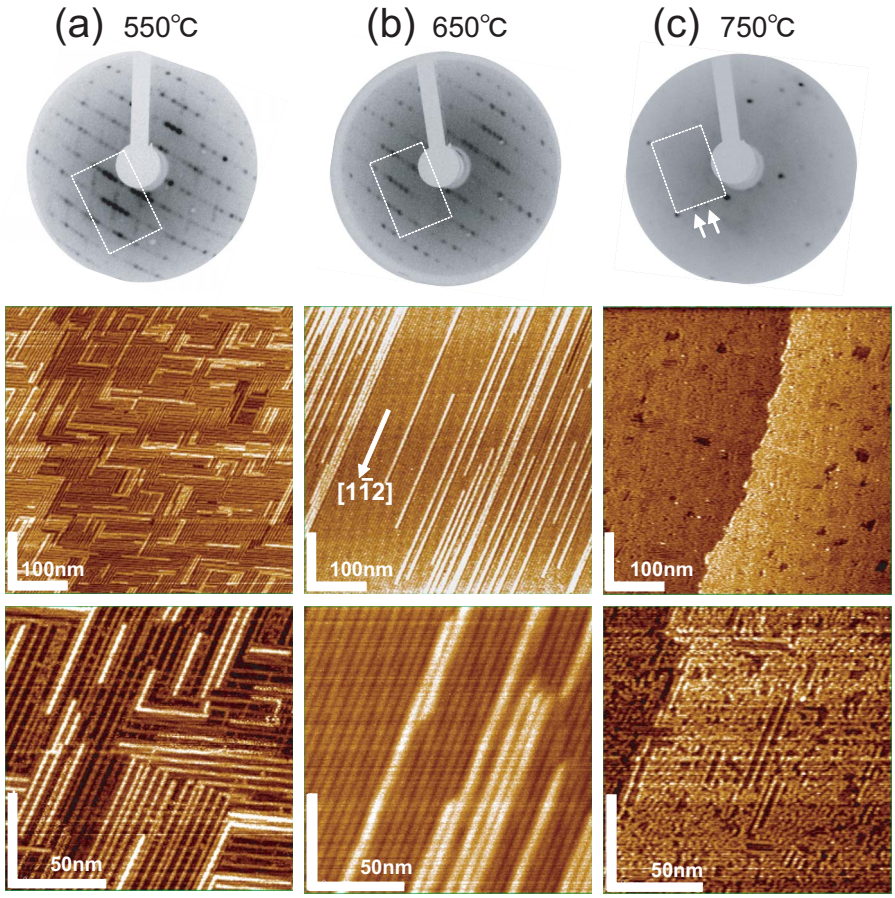

FIG. 2. (Color online) LEED and STM images of the surfaces after 30 min annealing at (a) 550 °C, (b) 650 °C, and (c) 750 °C, with the dc along [1 −12]. LEED patterns are recorded at incident beam energy of 65 eV. STM image is obtained in constant-current mode with sample bias voltage of 1 V. Sizes of STM images are 500 $\times$ 500 nm^2 (top) and 150 $\times$ 150 nm^2 (bottom).

utilize in this study is dc electric current and field. Since the surface atoms of Si(110) are known to donate charges to the underneath atoms as in the case of other faces,[6] they are an object of the electromigration.[10–13] In this Brief Report, we show a simple surface preparation method for the single-domain of Si(110)-16$\times$2 utilizing the electromigration. The electromigration of surface atoms upon the resistivity heating by dc (dc heating) is shown to play a critical role in the formation of the 16$\times$2 reconstruction. By means of a controlled electromigration, we fabricated a micrometer-wide single domain of the 16$\times$2 structure with nearly perfect reproducibility.

A medium-doped n-type Si(110) of 0.5–1.5 Ω cm has been used for the specimen. The 0.3-mm thick wafer is cut into $1\times\bar{7}$ mm^2, in two different orientations for the long side, [1$\bar{1}$2] and [1$\bar{1}$0] as shown in Fig. 1(c). The sample surface was prepared in UHV by the dc heating, with the current along the long side of the specimen. This allows us to examine two different dc directions with respect to the orientation of the 16$\times$2 reconstruction: along one reconstruction row ([1$\bar{1}$2]) and in between the rows ([1$\bar{1}$0]). The sample was degassed at around 150 °C for 7 h after being introduced to the UHV system. It was further degassed by repeated flash heating at 1200 °C. The 16$\times$2 reconstructed surface was prepared by prolonged annealing followed by quenching to room temperature. The annealing temperature and the current direction are the main parameters for surface preparation examined in this work. Note that the critical temperature (T_c) of the surface phase transition, the low-temperature 16$\times$2 phase to the high-temperature 1$\times$1 phase, is around 730 °C.[14,15] A temperature gradient within the sample during the dc heating is minimized as much as possible. All the annealing procedures were carried out in the pressure below 1×10^{-7} Pa. The surface structure after each preparation was checked with low-energy electron diffraction (LEED) and scanning tunneling microscopy (STM) at room temperature.

Figures 2 and 3 display a set of LEED and STM images of the surfaces prepared with dc in the [1$\bar{1}$2] and the [1$\bar{1}$0] directions, respectively. The direction of the current is parallel to the 16$\times$2 rows in the case of Fig. 2, while it is in between the rows in Fig. 3. Three different annealing temperatures with respect to T_c, (a) 550 °C, (b) 650 °C, and (c) 750 °C, have been examined. The annealing time is fixed to 30 min in all the cases. The current densities corresponding to three temperatures are (a) 0.3, (b) 0.7, and (c) 1.3 A/mm^2, respectively. First of all, the difference in appearance of surfaces shown in Figs. 2 and 3 is significant. In Fig. 2, annealing with temperatures below T_c [(a) and (b)] results in a characteristic stripe of 16$\times$2 throughout the surface, whereas surface is dominated by a disordered area in Fig. 3. This definitely indicates the relevance of the current direction in the dc heating process, which has not been considered so far.

We start the discussion with the most successful preparation shown in Fig. 2(b). The LEED image clearly shows the diffraction pattern from a single domain of the 16$\times$2 structure. It is confirmed that almost all the parts of the specimen

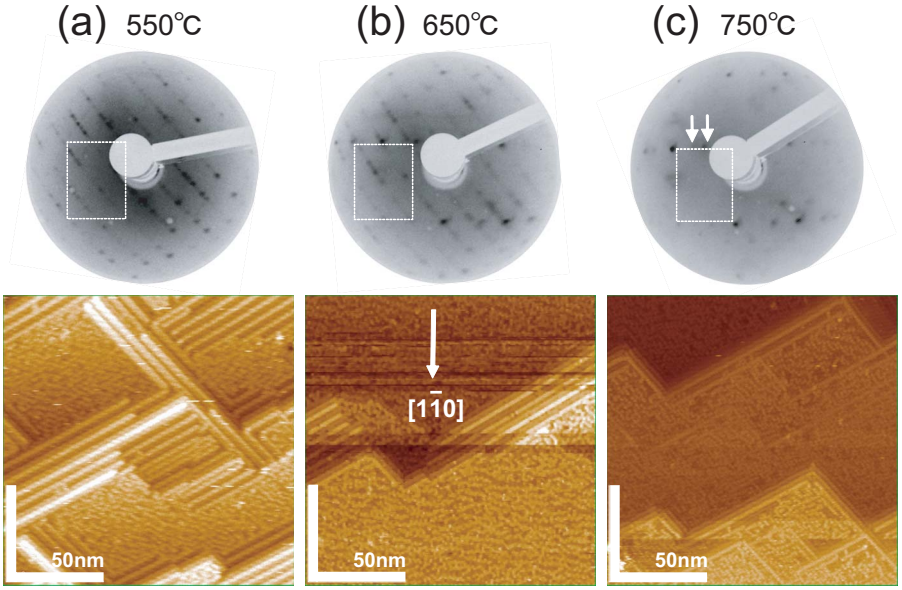

FIG. 3. (Color online) LEED and STM images of the surfaces after 30 min annealing at (a) 550 °C, (b) 650 °C, and (C) 750 °C, with the dc along [1$\bar{1}$0]. LEED patterns are recorded at incident beam energy of 65 eV. STM image is obtained in constant-current mode with sample bias voltage of 1 V. Size of STM image is 150×150 nm^2.

shows the same diffraction pattern, suggesting a formation of huge single domain over a millimeter size. STM image reveals that all the terraces show a striped structure of 16×2 only in the [1$\bar{1}$2] direction with few numbers of disorders. In contrast to the previous reports, many of the rows extend much more than 500 nm without a fragmentation. As far as we confirmed with the wide STM scans, similar domain extends at least over several dozens of μm^2 wide, both parallel and perpendicular to the rows. The formation of the so-called (17, 15, 1) step[14] (corresponding to the bright lines in STM) is rather random, which is uncontrollable at the moment. The single-domain surface as shown here has never been reported previously, at least in the real space. Although some authors have already found the formation of the single domain of 16×2 by LEED observations,[9,16] no explanation on the formation mechanism has been argued so far. In the following, we argue on the origin of the formation of the single domain based on the results from different preparations.

Annealing with lower temperature results in a well-known double-domain structure. As shown in Fig. 2(a), LEED pattern represents the diffraction from double domain of 16×2 structure. Note in the present case that the diffraction from one domain is stronger than the other, which will be discussed later. STM reveals a fragmentation of 16×2 rows and a formation of two domains with increased amount of disorders. Note also that one domain along [1$\bar{1}$2] is found to be more popular than the other domain, which is consistent with the LEED observation. The formation of the single domain at higher temperature (but below T_c) can be interpreted in two different ways: (1) The single domain is the ground state of the 16×2 reconstruction. (2) The single domain is a metastable phase that happened to be stabilized. For anisotropically strained one-dimensional structure such as the 16×2 reconstruction, scenario (1) should be less likely. We could rather reasonably assume the more isotropic double domain to be the ground state below T_c. Then, the formation of the metastable single domain indicates the existence of one more factor other than temperature to be considered in the reconstruction process upon the dc heating. This factor should be the electromigration of the surface atoms.

Figure 3 displays the sets of surfaces prepared with the same heating procedures as tried in Fig. 2, but in a different current direction ([1$\bar{1}$0] in between the reconstruction rows). The resulting surfaces in this case are very different from those in Fig. 2. Even after the annealing at 650 °C, which was the best condition in the case of Fig. 2, the LEED pattern displays only weak diffraction due to 16×2 reconstruction together with also weak 5×1 superstructure characterized by fractional spots along the [001] direction[17] (not very clear in the LEED picture at that incident beam energy). STM reveals the presence of the large amounts of disordered structure instead of the 16×2 structure. The fractions of the 16×2 line can only be seen at the step edges. This observation is also considered to be unusual because of the fact that the ground state (16×2 structure) has not been reached despite the annealing with an adequate temperature. Annealing with lower temperature [Fig. 3(a)], on the other hand, causes the increase in the 16×2 parts. STM measurement confirms the increased 16×2 regions around the step edges in two directions, although the disorderlike area is still noticeable. LEED also confirms the presence of 5×1 diffraction spots together with rather clear 16×2. It is found that in order to make the most of the surface into 16×2, much more prolonged annealing (1–2 h) is required. Again, these observations are in strong contrast with those shown in Fig. 2.

The strict different tendency between Figs. 2 and 3 helps us to figure out the rule of the electromigration in the 16×2 formation. Present results clarify that the dc along [1$\bar{1}$2] tends to line up the 16×2 rows, while that in the [1$\bar{1}$0] direction prevents the formation of 16×2. This can be almost straightforwardly understood in terms of the electromigration; the diffusion of the adatoms along the rows helps to elongate the reconstruction lines, while the diffusion not parallel to it causes a fragmentation of rows. Similar observation has been made in the vicinal Si(111) surface, where the dc parallel to the step is found to move the kinks along the step edges forming the straight steps.[11–13]

In sample heating with dc, the effects from the isotropic

thermal annealing and the anisotropic electromigration always coexist inevitably. It should be the competition of these effects that determines the resultant structure. At the higher temperature where the diffusion is promoted, the electromigration effect becomes noticeable. This elongates the reconstruction line along the direction of the current resulting in the single domain when the current direction matches the orientation of the rows. On the other hand, at the lower temperature, a limited diffusion reduces the effect of the electromigration, resulting in the random distribution of short rows, which forms the stable double domain regardless of the current direction. However, it is noted that the electromigration is still effective even in the cases of Fig. 2(a) and 3(a). The remaining effect of the electromigration explains why the intensity of one domain is stronger than the other in Fig. 2(a) and why there exist so many disorders in Fig. 3(a). It should be emphasized that the reproducibility of the preparation of the single domain is almost 100% in our condition. In addition, the single domain and the double domain can controllably be fabricated in a reversible manner. The optimum parameter for the dc heating, however, should be different from system to system depending on the sample shape and resistivity.

Finally, the 5×1 and the disordered structure found together with 16×2 are discussed briefly. The disordered structure seen in Fig. 3 is known to be a disordered arrangement of the building blocks for 16×2 structure reported as "pair of pentagons" (PP).[7,18] PP is also known to be the building block for the 5×1 structure.[7,19] The observed fact that the surface with large amount of the disordered PP (Fig. 3) produced the 5×1 and 16×2 diffraction agrees with the above arguments. The PP structure is so stable that the surface is always covered with it even after quenching the surface from the high-temperature 1×1 phase, regardless of the current directions as shown in Figs. 2(c) and 3(c). LEED also confirms the presence of clear 5×1 diffraction spots (indicated by arrows) in quenched surface instead of perfect 1×1. This suggests the high stability of the PP structure even at high temperature comparable to T_c. It can be assumed that, below T_c, the electromigration helps to diffuse and align the PP unit in the 16×2 position when the current direction matches the reconstruction row, while other current directions cause rather random arrangement of the PP producing the 5×1 diffraction. It is noted that the 5×1 is also stabilized by very small amounts of impurity such as Ni.[18,20] In our case, however, both 16×2 and 5×1 can be selectively formed on the same sample, which is contrary to the case of the Ni-induced 5×1 structure,[18] where 5×1 cannot be removed only by annealing.

In conclusion, it is shown that the electromigration of the surface atoms, which has not been considered so far for Si(110), has a remarkable effect on the surface reconstruction process. By utilizing the electromigration along the $[1\bar{1}2]$ direction, a micrometer-wide single domain of 16×2 can be fabricated reproducibly. Depending on the condition of the electromigration, a common double domain of 16×2 can also be formed. Both single- and double-domain structure can be fabricated selectively in a reversible manner. The well-established surface preparation method for clean single domain of Si(110) can be utilized in future investigations of the basic surface properties such as the electronic structures or the surface reaction. In addition, the strong one dimensionality of the wide single domain of 16×2 has high potential for applications. The fabricated single domain of 16×2 reconstruction is actually a pile of the straight monatomic steps. This implies a promising application of this surface as another type of template for one-dimensional functional nanostructures such as atomic and/or molecular wires.

This work was partially supported by the Ministry of Education, Science, Sports, and Culture, Grant-in-Aid for Young Scientists (start-up), 18810041, 2007. One of the authors (A.G.) would like to thank Région Rhône-Alpes, France, for financial support.

[1] T. Sato, Y. Takeishi, H. Hara, and Y. Okamoto, Phys. Rev. B **4**, 1950 (1971).
[2] A. Ciucivara, B. R. Sahu, S. Joshi, S. K. Banerjee, and L. Kleinman, Phys. Rev. B **75**, 113309 (2007).
[3] M. Suemitsu, A. Kato, H. Togashi, A. Konno, Y. Yamamoto, Y. Teraoka, A. Yoshigoe, Y. Narita, and Y. Enta, Jpn. J. Appl. Phys., Part 1 **46**, 1888 (2007).
[4] S. Liang, R. Islam, D. J. Smith, P. A. Bennett, J. R. O'Brien, and B. Taylor, Appl. Phys. Lett. **88**, 113111 (2006).
[5] Y. Liu, K. Ishii, T. Tsutsumi, M. Masahara, T. Sekigawa, K. Sakamoto, H. Takashima, H. Yamauchi, and E. Suzuki, IEEE Trans. Nanotechnol. **2**, 198 (2003).
[6] A. A. Stekolnikov, J. Furthmuller, and F. Bechstedt, Phys. Rev. Lett. **93**, 136104 (2004).
[7] T. An, M. Yoshimura, I. Ono, and K. Ueda, Phys. Rev. B **61**, 3006 (2000).
[8] See, for example, tables in Y. Yamamoto, Surf. Sci. **313**, 155 (1994).
[9] N. D. Kim, Y. K. Kim, C.-Y. Park, H. W. Yeom, H. Koh, E. Rotenberg, and J. R. Ahn, Phys. Rev. B **75**, 125309 (2007).
[10] M.-S. Ho, I.-S. Hwang, and T. T. Tsong, J. Appl. Phys. **97**, 023522 (2005).
[11] S. Yoshida, T. Sekiguchi, and K. Ito, Appl. Phys. Lett. **87**, 031903 (2005).
[12] Y.-N. Yang, E. S. Fu, and E. D. Williams, Surf. Sci. **356**, 101 (1996).
[13] A. Kirakosian, R. Bennewitz, J. N. Crain, Th. Fauster, J.-L. Lin, D. Y. Petrovykh, and F. J. Himpsel, Appl. Phys. Lett. **79**, 1608 (2001).
[14] Y. Yamamoto, T. Sueyoshi, T. Sato, and M. Iwatsuki, Surf. Sci. **466**, 183 (2000).
[15] W. Swiech, T. S. Selinger, and D. G. Cahill, Surf. Sci. **519**, L599 (2002).
[16] H. Ampo, S. Miura, K. Kato, Y. Ohkawa, and A. Tamura, Phys. Rev. B **34**, 2329 (1986).
[17] E. G. Keim, H. Wormeeter, and A. Silfhout, J. Vac. Sci. Technol. A **8**, 2747 (1990).
[18] M. Yoshimura, Surf. Sci. **433-435**, 470 (2000).
[19] W. E. Packard and J. D. Dow, Phys. Rev. B **55**, 15643 (1997).
[20] T. Ichinokawa, H. Ampo, S. Miura, and A. Tamura, Phys. Rev. B **31**, 5183 (1985).