Single-Domained Si(110)-“16x2” Surface

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Abstract. Micrometer-wide, single-domain of 16x2 reconstruction, the array of straight monoatomic steps, has been fabricated on Si(110) surface by means of controlled electromigration of surface atoms. The electromigration effect during DC current heating is found to line-up the reconstruction rows when the current direction matches to the direction of the rows. This provides not only a well-controlled surface preparation method for Si(110), but also a new template for low-dimensional nanostructures.

1. Introduction
Si(110) surface is currently attracting renewed interests because of its unique properties such as high hole mobility [1, 2, 4], peculiar surface reactivity [3], and strong morphological anisotropy [5]. However, despite of the increasing requirements, the number of studies on the Si(110) surface has been surprisingly small and many basic properties including surface atomic structure remain unsolved. The delay of the studies on the Si(110) surface is partly due to a difficulty in the surface preparation. The clean Si(110) surface has a complicated surface reconstruction with huge unit cell, namely “16x2” reconstruction as shown in fig.1. Typically reported surfaces exhibits a double-domain structure of “16x2” reconstruction identified with fragmented rows running along two directions, [1-12] and [-112]. In addition, a disorder-like structure always coexists with the double domain of “16x2”. Furthermore, various surface reconstructions other than “16x2” due to small amounts of impurities have been found, suggesting the instability of the “16x2” structure. So far, the inhomogeneity and instability of the surface reconstruction have hindered a detailed determination of the properties of Si(110) such as surface electronic structure and surface chemical reaction, as well as structural determination. For further development of the understanding of Si(110), it is quite important to establish the preparation method for well-defined, single-domain surface of Si(110).

In this paper, we show a simple surface preparation method for the large single-domain of Si(110)-“16x2” utilizing the electromigration [10]. The electromigration of surface atoms upon DC current heating is shown to play a critical role in the formation process of “16x2”. By means of the controlled electromigration, we were able to fabricate a micrometer-wide, single-domain “16x2” structure with nearly perfect reproducibility.

2. Experimental
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 used is cut into 1x7 mm², in two different orientations for the long side, [1-12] and [001], as shown in fig.1. The sample surface was prepared by a resistivity heating by the DC current with the
current direction along the long side. This allows us to examine different heating current directions with respect to the “16×2” structure; along one reconstruction row ([1-12]) and in-between the rows ([001]). The sample was degassed at around 150 °C for 7 hours after introducing to the UHV system. It was then flash-heated for several times at 1200 °C for further degassing. The “16×2” surface was prepared by the annealing at certain temperature for 30 min, followed by quenching to RT. The annealing temperature and current direction are main parameters for surface preparation examined in this work. The important temperature here is the critical temperature of the phase transition (Tc), the LT “16×2” phase to the HT 1×1 phase, which has been reported to be around 730 °C. All the annealing procedure was 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 microscope (STM) at room temperature.

3. Results and discussion

Fig.2 and 3 display the set of LEED and STM images of the surface prepared with DC current in [1-12] and [001] direction, respectively. The direction of the DC current in the case of fig.2 is parallel to the one reconstruction row, while it is in-between rows in fig.3. Three different annealing temperatures with respect to Tc have been examined in each case, (a) 600 °C, (b) 700 °C, and (c) 800 °C. The annealing time is fixed to 30 minute. The current density corresponding to each preparations are (a) 0.3, (b) 0.7, and (c) 1.3 A/mm², respectively. First of all, it is clearly found that the appearances of the surfaces after annealing with temperatures below Tc are completely different depending on the current direction. This indicates the strict relevance of the current direction in the resistivity heating process, which has not been considered so far for this surface. We start the discussion with results from the most successful preparation, which is Fig.2 (b). The LEED image in fig.2-(b) clearly shows the diffraction pattern from a single-domain of “16×2”. STM observations reveal that all the terraces show a striped structure of “16×2” in [1-12] direction with few numbers of disorders. Figure 4 displays the wide scan of the single-domain. Many of the rows are found to extend much more than 500 nm without fragmentation. The single-domain extends at least several dozens of μm² wide. On the other hand, annealing with lower temperature yields the double-domain structure, as shown in fig.2-(a). Note in the present case, the domain along [1-12] is found to be more popular than the other domain, which will be discussed later.

The surfaces in fig.3 are very different from those in fig. 2. After the annealing at 700 °C, fig. 3 (b), the LEED pattern displays only very weak diffraction due to “16×2” reconstruction together with also very weak “5x1” superstructure. STM reveals that the most parts of the surface in this case are in a disorder-like structure instead of the “16×2”. Annealing with lower temperature (fig. 3-(a)) causes the increase in the double-domain of the “16×2”. STM measurement confirms the increased “16×2” regions around the step edges in two directions, along [1-12] and [-112], although the disorder-like area is still dominant. It is found that in order to make the most of the surface into “16×2”, the prolonged annealing with even lower temperature (1-2 hours, around 550 °C) is required.

The strict different tendency between fig.2 and 3 helps us to figure out the rule of the electromigration in the “16×2” formation. Present results clarify that the DC current along [1-12] tends to line-up the “16×2” rows, while that in [001] 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 breaks the rows. Quite similar observations have been made in the vicinal Si(111) surface, where the DC current is found to manipulate step structure. In the resistivity heating with DC current, isotropic thermal annealing and anisotropic electromigration always coexist. It should be a competition of these effects that determine the resultant structure. At the higher temperature where the input power is also high, the electromigration along the direction of the current overwhelms the isotopic thermal annealing. Thus the single-domain (in the case of fig.2-(b)) or the disorder-like structure (fig.3-(b)) are formed depending on the current direction. On the other hand, at the lower temperature where the electromigration is weak and the isotopic thermal annealing becomes dominant, the surface tends to...
form the stable double-domain structure regardless of the current direction. For the present case, however, the electromigration is considered to be still effective even in the case of 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 disorder-like structures 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 disorder-like structure seen in fig.2-(a) and fig. 3-(a, b) is known to be a disordered arrangement of the building block for “16×2” structure, reported as “pair of pentagon (PP)”\textsuperscript{7,17}. It is also known that this structure is also building block for the “5×1” structure.\textsuperscript{7,14} The PP structure is so stable that the surface almost covered with it even after quenching from HT-1×1 phase, confirmed in figs 2-(c) and 3-(c). LEED indicates a weak “5×1” and very weak “16×2” (double-domain), possibly caused by short range ordering of PP. It can be assumed that below Tc, the electromigration helps to align the PP in the “16×2” fashion when the current direction matches the reconstruction row, while other current directions causes disordered arrangement of the PP.

In conclusion, it is shown that the electromigration of the surface atoms has a remarkable effect on the surface reconstruction process. By utilizing the electromigration along [1-12] direction, a micrometer-wide single domain of “16×2” can be fabricated reproducibly. Depending on the strength and direction of the electromigration, a common double-domain of “16×2” can also be formed. 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 electronic structures or surface reactivity. On the other hand, the strong one-dimensionality of the wide single-domain of “16×2” has high potential for applications. The “16×2” reconstruction is a pile of the straight monoatomic steps. This implies a promising application of this surface as a new template for one-dimensional functional nanostructures such as atomic/molecular wires.

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Fig. 1  Schematic drawings of (a) surface atomic structure with 2 equivalent unit cells for “16×2” reconstruction (red and blue), (b) 2 specimens with different orientation used in this study, (c) reciprocal lattice scheme for “16×2” reconstruction.

Fig. 2  LEED and STM images of the surfaces after annealing of (a) 600 °C, (b) 700 °C, (c) 800 °C, with the DC current along [1-12] direction. LEED patterns are obtained at incident beam energy of 65 eV. STM image is recorded in constant-current mode with sample bias voltage of 1 V. The size of STM images is 150×150 nm².

Fig. 3  LEED and STM images of the surfaces after annealing of (a) 600 °C, (b) 700 °C, (c) 800 °C, with the DC current along [001] direction. LEED patterns are obtained at the incident beam energy of 65 eV. STM image is obtained in same conditions as for fig.2. The size of STM images is 200×200 nm². (150×150 nm² for (c)).

Fig. 4  1μm × 1μm-STM image of single-domain of Si(110) surface fabricated by controlled electromigration.