One-Dimensional Nanotemplate Structure of a Si(110) Substrate*

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The process for the formation of a single-domain one-dimensional nanotemplate with a 16×2 reconstruction was investigated via scanning tunneling microscopy. Si(110) substrates with different resistivities were heated with direction-controlled direct currents. It was determined that obtaining a single-domain 16×2 reconstructed structure for a substrate with a lower resistivity even at the same annealing temperature is time consuming, which indicates that applied voltage rather than current flow plays a dominant role in single-domain formation.

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I. INTRODUCTION

Recently, the Si(110) surface has attracted significant interest as a candidate for next-generation semiconductor devices because of its high hole mobility compared with that of other low-index Si surfaces [1–3]. At the same time, it is also known that Si(110) has a unique one-dimensional (1-D) 16×2 reconstructed structure [4–7]. The 16×2 reconstructed structure shows alternate stripes of up and down atomic steps that consist of surface adatom units (pairs of pentagons; PPs). This unique 1-D striped structure can be used as a nanotemplate for low-dimensional nanostructures. However, the clean Si(110)- 16×2 structure usually exhibits a double-domain structure, where the 16×2 structures run along two equivalent directions of $[\bar{1}12]$ and $[1\bar{1}2]$. Moreover, various reconstructed structures other than the 16×2 structure are formed owing to the presence of small amounts of impurities. Thus, the controlled synthesis of 1-D nanostructures using the 16×2 nanotemplate has not yet been achieved.

Yamada *et al.* reported that a well-defined single-domain 16×2 structure can be fabricated by means of direction-controlled direct current (DC) heating [8]. DC heating can induce the electromigration (EM) of surface Si atoms in order to line up the reconstruction rows when the DC direction matches the orientation of the rows. That is,

FIG. 1: (a) STM and LEED images of the clean Si(110)- 16×2 single-domain surface ($1 \mu\text{m} \times 1 \mu\text{m}$, $V_s = 2.0 \text{ V}$) and (b) magnified STM image ($30 \text{ nm} \times 30 \text{ nm}$) shown in Fig. 1(a). The Si atoms that constitute PPs are resolved (inset of (b)).

EM on semiconductor surfaces is effective for mass transport toward either the cathode or anode over the surface at a sufficiently high temperature. It is known that EM apparently depends on annealing temperature, time, density of current flow, electric field, and DC direction [9–17]. However, the dominant driving force of EM for Si(110)- 16×2 single-domain formation has not been clarified yet.

To elucidate the essential driving force of EM, it is necessary to investigate the dependence of EM atom movement on current flow and applied voltage. In this study, we fabricated a single-domain 16×2 reconstructed structure on Si(110) substrates with different resistivities and reveal that applied voltage is the dominant parameter that drives EM.

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FIG. 2: Changes in the surface structure of the LR Si(110) with increasing DC heating time at 873 K. To obtain the single-domain 16×2 surface, it was found that prolonged annealing at 873 K was required.

II. EXPERIMENTAL

Experiments were conducted using an ultrahigh vacuum scanning tunneling microscopy (STM) (JSPM 4500A, JEOL Ltd.) system equipped with molecular deposition sources and low-energy electron diffraction (LEED) optics. The base pressure in the measurement chamber was $\sim 2 \times 10^{-8}$ Pa. In this study, a high resistivity (HR) Si(110) substrate (resistivity; $0.5\text{--}1.5 \, \Omega \text{ cm}$) and a low resistivity (LR) Si(110) substrate (resistivity; $0.01\text{--}0.02 \, \Omega \text{ cm}$) were used. All STM measurements were performed at room temperature (RT).

III. RESULTS AND DISCUSSION

To fabricate the single-domain 16×2 structure on an HR Si(110) substrate, DC flowing along the $[\bar{1}12]$ direction was used to heat the surface at 1500 K for 30 s, followed by prolonged annealing at 873 K for 20 min and then quenching to RT. The STM and LEED images of the sample obtained using this procedure are shown in Figs. 1(a) and (b). Figure 1(a) clearly shows that a single-domain structure is formed over $1 \, \mu\text{m}^2$ with stripes that run along the DC direction. The inset LEED image consists of the spots originating from the single-domain 16×2 reconstruction. The rectangle in the LEED image indicates a 1×1 unit cell. Because the same LEED images were obtained throughout the specimen, it was determined that the single-domain 16×2 structure was formed over the entire specimen. In the magnified STM image shown in Fig. 1(b), the Si atoms that constitute PPs are resolved. The spacing between the adjacent stripes is approximately 5 nm and the height of each stripe is approximately 0.2 nm, which agree with previously reported results [5].

However, for the LR Si(110) specimen, the single-domain 16×2 structure was not obtained when the same procedure as that described above for the HR Si(110) was employed. Figure 2(a) shows the STM image of the surface after 30 s of flashing at 1500 K followed by 20 min of annealing at 873 K. The surface appears to have a disordered structure. However, it is not really disordered, but has a short range ordering of PPs. Although the LEED image is indistinct, the spots reflecting this short range order can be identified. Moreover, the partly formed striped structures at the step edge suggested that a longer annealing time at 873 K is required to expand the area of the ordered structure. Figures 2(b)-(f) show the changes in the surface morphologies that occur with increased annealing times at 873 K. In Figs. 2(b) and (c), the apparent disordered terrace structures are slightly ordered and the step structure is straight. In Figs. 2(d) and (e), the 16×2 structures is gradually extended from the step edge to the inner terrace and almost the entire surface is covered with the 16×2 structure after annealing for 8 h. However, another directed domain has begun to form at the step edges. Finally, after overnight annealing for approximately 14 h, the single-domain 16×2 structure (Fig. 2(f)) is achieved throughout the specimen, as can be seen in the LEED image. Therefore, it was clearly demonstrated that the 16×2 single-domain formation of the LR Si(110) substrate requires an extended period of DC heating at 873 K. Note that single-domain formation for the LR Si(110) does not necessarily require 840 min of annealing at 873 K. Depending on the sample, it is possible to form the single domain with a shorter annealing time. This variation in the required annealing time suggests that surface conditions such as cleanliness and flatness of the original substrate, the deviation of dopants, and the pressure during annealing differ slightly with each sample. However, it is not possible to form the single-domain 16×2 struc-

FIG. 3: (a) Current-temperature and (b) voltage-temperature features for the two Si(110) substrates with different resistivities.

TABLE I: Summary of single-domain formation on the two Si(110) substrates with different resistivities (the required annealing time in the last row is the time required to achieve the single-domain 16×2 structure with annealing at 873 K).

	Low resistivity Si(110)	High resistivity Si(110)
Resistivity [Ωcm]	0.01-0.02	0.5-1.5
Current density [A/cm^2]	132	67
Electric field [kV/m]	0.5	1.2
Required annealing time [min]	840	20

ture by annealing for 20 min, such as is the case for HR Si(110). These results suggest that the efficiency of EM differs between the two Si(110) specimens with different resistivities.

Figures 3(a) and (b) show the current-temperature and voltage-temperature features for the two Si(110) specimens, respectively. The temperature dependence of both current and voltage at higher temperatures show the same trends for the two specimens because the difference in resistivity almost disappears at higher temperatures, where the carriers are thermally excited beyond the band gap. On the other hand, a difference in the temperature dependence of the two specimens arises below 1200 K. To extend the single-domain areas in the HR Si(110) by annealing at 873 K, a current of 0.2 A and an applied voltage of 8.5 V are required corresponding to a current density of $67 \text{ A}/\text{cm}^2$ and an electric field of 1.2 kV/m. However, in the case of the LR Si(110), 0.5 A and 3.8 V are required corresponding to a current density of $132 \text{ A}/\text{cm}^2$ and an electric field of 0.5 kV/m. These values are summarized in Table I. Although a higher density current flow is used for the LR Si(110) than that for the HR Si(110), single-domain formation requires a much longer annealing time at 873 K. In other words, in the case of the HR Si(110) specimen, a larger electric field enables shorter annealing time even at the same temperature.

Generally, the EM of atoms is described in terms of the electric wind force model [15, 16]. In this model, because the number of electrons that collide with an atom, or current density, acts as the driving force for EM, it increases with current density. Nevertheless, it has been reported that the electrons involved in the collisions must have a critical energy in order to cause the EM of metal atoms [18]. Therefore, EM should not readily occur in substrate with a low applied voltage.

Of course, various other factors act reciprocally on EM.

For example, a different surface temperature results in a different EM speed. However, the temperature range at which the Si(110)- 16×2 single domain can form is very limited. Therefore, in this study, surface temperature was maintained at approximately 873 K and applied current, voltage, and required annealing time for Si(110) substrate with different resistivities were measured. Based on the results from these experiments, it was concluded that for Si(110), applied voltage rather than flow of current is a dominant driving force for EM leading to single-domain formation. It is expected that these findings will be useful for the fabrication of a new nanotemplate structure.

IV. CONCLUSIONS

We have investigated the process for the formation of a single-domain 16×2 structure on Si(110) specimens with high and low resistivities using DC heating. Single-domain 16×2 formation on the LR Si(110) specimen requires an extended annealing time at 873 K despite the higher density of current flow. This result indicates that for Si(110)- 16×2 single-domain formation at an annealing temperature of 873 K, applied voltage rather than flow of current is a dominant driving force for EM.

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