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Step bunching and step "rotation" in homoepitaxial growth of Si on Si(110)-16×2

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ABSTRACT

Kinetics of the step flow growth on the (16×2) reconstructed Si(110) surface has been studied experimentally and with computer simulations. It is shown that during Si growth under DC heating vicinal steps on the (16×2) reconstructed Si(110) surfaces undergo a kinetic step bunching and develop extended segments preferentially oriented along the (16×2) reconstruction domains. The final step configuration depends crucially on the direction of the applied electric field. In particular, when DC is applied in the $[1\bar{1}2]$ direction, an array of straight multisteps parallel to the current direction and rotated in respect to the original orientation of the vicinal steps can be fabricated. Surprisingly, the observed step transformations are not affected by the polarity of the applied electrical field. Using a simple model of the Si/Si(110)-(16×2) growth and kinetic Monte Carlo simulations we show that the step bunching and step rotation on Si(110)-(16×2) might be induced by an incoherent matching of the (16×2) reconstruction domains across the vicinal steps on the surface.

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1. Introduction

Stepped crystalline surfaces are of great importance for modern semiconductor science and technology. They are commonly considered as useful templates for fabrication of various nanostructures. For instance, arrays of regularly spaced monoatomic steps provide natural templates for growth of spatially uniform epitaxial nanowires and nanostripes [1–4], while multisteps, or step-bunches, can be used to fabricate ordered arrays of quantum dots [5–9]. On the other hand, observations of the step behavior supplemented by an appropriate theoretical treatment may provide valuable information on the atomic scale surface processes hardly accessible by other means [10].

Among other low index silicon surfaces the Si(110) surface is becoming increasingly important for microelectronics. This surface orientation shows superior hole mobility compared to conventional Si (001) [11]. Also strong structural anisotropy of Si(110) is considered to be very promising for fabrication of one-dimensional nanostructures [12–14]. To add to that, Si(110) has recently been proven to be a good starting substrate for forming graphene-on-silicon (GOS) structures [15–17].

To take full advantage of Si(110), however, preparation of high quality Si(110) surfaces with well defined step morphology is indispensable. In that respect the Si(110) surface represents a complicated case. Indeed, at temperatures below 730 °C the clean Si (110) surface is characterized by the (16×2) reconstruction, which consists of a sequence of alternating 2.5 nm-wide up and down terraces separated by monoatomic steps [18,19]. This is in sharp contrast to the Si(001) and Si(111) surfaces where the presence of the steps is conditioned solely by the surface miscut and nucleation of two-dimensional islands. On Si(110), therefore, the steps represent essential building blocks for the surface reconstruction. This fact has a great impact on the homoepitaxial growth on Si(110) and, as we will show in the present paper, makes the surface inherently unstable against step bunching.

In addition to the (16×2) structure, fragments of the (17,15,1) facets are frequently observed on Si(110) [19,20]. The atomic structure of the (17,15,1) planes is similar to the (16×2) structure, except for the replacement of the up-down sequence of the 2.5 nm-wide terraces in (16×2) with a sequence of either up-up-... or down-down-... terraces in (17,15,1). The (17,15,1) facets thereby represent the edges of multisteps [21]. The (16×2) structure transforms into a disordered (1×1) structure at temperatures above 730 °C and the (17,15,1) step structure disappears completely above 770 °C, leaving only fluctuating vicinal steps on the surface [22,23].

The fact that these structural transitions are reversible [22,23] suggests that the (17,15,1) steps may have formed by spontaneous alignment of fluctuating vicinal steps during the slow cooling down passage across the critical temperatures (770 °C) after, say, a high temperature oxide removal in vacuum [24]. Rapid quenching of high-temperature treated samples, on the other hand, prevents formation

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of such step bunches [23]. Therefore, tuning of the thermal treatment provides a possible, if not overwhelming, way to control the step configurations on the Si(110) surface.

Another, and somewhat more flexible, method to control the steps on Si(110)-16×2 is to use direct electric current (DC) for heating the substrate. Generally, the Si(110)-16×2 reconstruction occurs in two randomly distributed domains, formed by the atomic steps oriented along either $[\bar{1}12]$ or $[1\bar{1}2]$ directions. Recently, Yamada et al. [25,26] have demonstrated that a single-domain Si(110)-16×2 surface can be prepared by DC annealing. In particular, by tuning the direction of the DC flow to either $[\bar{1}12]$ or $[1\bar{1}2]$ direction, either (16×2) or (2×16) single domain prevails. Little is known, however, about the impact of the DC heating of Si(110) on the growth, which is compared to Si (111) and Si(001) surfaces, where resistive substrate heating is widely used to tune the step pattern both under annealing [27–32] and during growth [33,34].

In the present paper we demonstrate that behavior of the surface steps on Si(110) can be controlled with the direction of the heating current. Specifically, growth of a 100 nm buffer layer on Si (110) under resistive DC heating in the $[00\bar{1}]$ direction results in appearance of zigzag shaped multisteps on Si(110). Silicon growth under DC flowing in the $[1\bar{1}2]$ direction, on the other hand, results in a regular array of rotated (17,15,1) steps with the edges parallel to the heating current direction. Surprisingly, the DC polarity shows only a minor effect on the resulting step pattern, suggesting that the step bunching on Si(110) is not provoked by the applied electric field but should be related to some intrinsic properties of this surface. Using kinetic Monte Carlo simulations we show that the step bunching on Si(110) is most likely to be induced by incoherent matching of the (16×2) reconstructed domains across the vicinal steps on the surface.

2. Experiment

Two sets of rectangular samples with the long edges parallel to <001> and <1$\bar{1}$2> directions were cut from a p-type Si(110) wafer as shown in Fig. 1(a). Samples were resistively heated by passing a DC along the long edge of the sample, so that we were able to explore two different current directions. Prior to Si growth, a standard ex situ wet chemical cleaning process with final dipping in HF was applied [35]. After introduction into the growth chamber, the samples were out-gassed in ultrahigh vacuum environment for 5 h at 550 °C, followed by flash-cleaning at 1200 °C for 30 s for several times. A 100-nm homoepitaxial Si layer was grown at a rate of 0.1 nm/s at a substrate temperature of 700 °C using gas-source molecular beam epitaxy with disilane (5×10^{-5} Torr) as a source gas. Temperature was monitored by an optical pyrometer. After the Si growth, samples were quenched to room temperature and transferred out from the UHV chamber. The surface morphology of the homoepitaxial layer was characterized by ex-situ atomic force microscopy (AFM) in air in the contact mode.

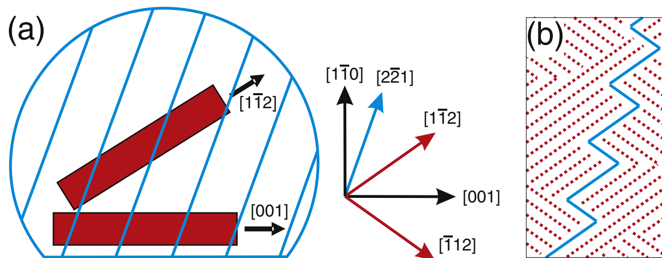

Fig. 1. (a) Two sample cuts used in this study. Thin straight lines indicate average orientation of the vicinal steps on the substrate surface. (b) Schematic representation of a double domain Si(110)-16×2 surface. Dotted lines show orientation of two (16×2) reconstruction domains. The solid line indicates the edge of a vicinal step running, on average, along the $[2\bar{2}1]$ direction.

Fig. 2(a) shows a typical AFM image of the Si(110) surface after UHV flash annealing at 1200 °C. The surface is relatively flat and smooth. Although we cannot identify individual vicinal steps in Fig. 2 (a), the absence of any step bunching is evident.

The morphology of the Si(110) surface changes drastically after growth of a 100 nm Si layer with the DC applied in the $[00\bar{1}]$ direction (Fig. 2(b)). As can be seen, the Si(110) surface undergoes a step bunching during growth, which leads to an array of multisteps on the surface. The multisteps are typically 5–6 atomic-layers high and their edges are on average oriented along the $[2\bar{2}1]$ direction.

While the average $[2\bar{2}1]$ orientation of the steps in Fig. 2(b) simply reflects the miscut direction of the original wafer, the step edges microscopically consist of a sequence of alternating low index segments. One possible combination is a pair of $[1\bar{1}2]$ and $[1\bar{1}\bar{1}]$ directed segments, which is suggested by the fact that the $[2\bar{2}1]$ index is a sum of the $[1\bar{1}2]$ and $[1\bar{1}\bar{1}]$ indices. Although this is indeed the case to some extent, the majority of the segments seen in Fig. 2(b) run parallel to either one of the two principal directions of the (16×2) reconstruction (i.e. parallel to either $[\bar{1}12]$ or $[1\bar{1}2]$ directions), as sketched in Fig. 1(b). We understand this dominance of the (16×2)-related steps in terms of the preferred formation of the (17,15,1) facets which minimize the energy of multisteps formed by the step bunching. Coarsening of the $[\bar{1}12]$ and $[1\bar{1}2]$ oriented segments leads to a local "rotation" of the step edges during growth, while the macroscopic orientation of the steps is preserved.

Reversing the current direction from $[00\bar{1}]$ (step up) to [001] (step down) produces only minor changes of the step pattern during the Si growth (not shown). To be accurate, the $[1\bar{1}2]$-oriented segments become even longer, exceeding the length of their $[\bar{1}12]$ and $[1\bar{1}\bar{1}]$ counterparts. It should be emphasized, however, that although the formation of elongated $[1\bar{1}2]$ step segments is promoted under a step-down current, the step bunching occurs for both directions of the heating current.

As we have seen, when we apply a <001> DC to heat the Si(110) substrate during growth, two processes take place: (a) step bunching and (b) local rotation of steps toward either one of the two (16×2)-related directions. Stimulated by the latter finding, we have investigated the impact of the DC along the $[1\bar{1}2]$ direction during growth. The effect of the DC applied along the $[1\bar{1}2]$ direction is quite drastic, as can be seen from the formation of a rather regular array of straight steps aligned along the current direction (Fig. 2(c)). The typical step height is 5–6 monolayers of silicon, demonstrating, again, the occurrence of the step bunching. In contrast to the step bands obtained under the DC//<001> heating in Fig. 2(b), the DC//$[1\bar{1}2]$ results in the formation of multisteps not only locally but macroscopically rotated toward the $[1\bar{1}2]$ direction. A close inspection of the surface terraces reveals that neighboring step bands are linked by monoatomic steps which run across the terraces and belong simultaneously to both of the neighboring step bands. These monoatomic steps are inclined to the multisteps and do not possess a regular shape. The inclined monoatomic steps help to maintain the overall sample misorientation, making possible the formation of an array of regular straight multisteps rotated from the original orientation of the vicinal steps on the surface. It should be emphasized that the same effect is observed also under a reversed heating current (not shown).

The occurrence of the step bunching both at step-up and step-down DC flows rules out the adatom electromigration effect [33] as the major driving force for the observed step instability. Therefore, the step bunching on Si(110) must be attributed to some intrinsic growth kinetics of the Si(110)-16×2 surface. In the following we shall see that the step bunching can be reproduced with a simple kinetic model, based on some basic experimentally-proven features of the Si/Si (110)-16×2 growth mechanism.

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