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How the Down Step Edges Influence Formation of the 7×7 Structure

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Summary: A surface that has wide terraces was fabricated by utilizing the step bunching phenomenon to study the effect of the down step edges on the formation of the 7×7 reconstruction. The surface with wide terraces was quenched through the 1×1–7×7 phase transition, freezing the formation process of the 7×7 reconstruction. On this surface, it became possible to investigate the influence of the down step edges on the formation of the 7×7 reconstruction because the influence of the upper step edge, which is located at the other side of the terrace, did not reach to the down step edge. A considerable decrease in the existence probability of the 7×7 reconstruction was observed near the down step edges. This decrease cannot explained by electromigration and steps advancement caused by the difference in adatom density between the 7×7 and disordered structure. Instead, we propose that the decrease in existence probability at down step edges is well explained by a simple topographic model assuming corner holes as the growth nuclei of the 7×7 domains.

Key words: Si(111), steps, 7×7, scanning tunneling microscopy, quench

Introduction

The formation process of the 7×7 structure of Si(111) is of interest both scientifically and technologically; therefore, extensive research has been carried out to study how and why the 7×7 reconstruction forms and stands as a stable structure (Kumamoto *et al*. 1996). Even though the complete atomic formation process remains unclarified, many studies show that the formation of the 7×7 structures is influenced by many factors, such as preannealing treatment, miscut degree of the substrate, and the residual gas of vacuum (Endo *et al*. 1995). To exemplify, it is reported that the 1×1–7×7 phase transition temperature is subject to the oxygen concentration in the surface region (Ohdomari 1992).

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Probably the best known factor that influences the formation of the 7×7 structure is the upper step edge. The upper step edge is well known to serve as a growth nucleus for the formation of the 7×7 reconstruction (Phaneuf *et al*. 1988). High temperature in situ scanning tunneling microscopy (STM) observations have revealed how the 7×7 domains form and grow from the upper step edge (Kitamura *et al*. 1991, Tokumoto and Iwatsukui 1993). This is explained by an easier formation of a corner hole at the upper step edge compared with the normal terrace, because the formation of the corner hole is the rate-limiting process for the formation of the 7×7 structure.

On the other hand, the influence of the down step edge on the formation of the 7×7 reconstruction has not been researched. This is partly because on a usual vicinal surface, once the 7×7 domain emerges at the upper step edge, it quickly grows through the terrace and reaches the down step edge, making it impossible to discriminate effects of the down step edge from other factors.

In this paper we report the manner in which the down step edge influences the formation of the 7×7 reconstruction. A surface with wide terraces exceeding 200 nm in width was fabricated by utilizing the step bunching phenomenon (Latyshev *et al*. 1989). The surface was quenched through the 1×1–7×7 phase transition temperature, freezing the formation process of the 7×7 reconstruction. We were able to study the influence of the down step edge on the formation of the 7×7 domain, because the influence of the upper step edge only reached 40 nm into the terrace (< 1/5 of the width of the terrace). A considerable decrease in the existence probability of the 7×7 reconstruction was observed near the down step edges. This decrease cannot be understood by electromigration and advancement of step caused by the difference in adatom density between the disorder and reconstructed area (Yang and Williams 1994). Instead, we report that the general trend toward decrease in probability could be understood by a simple topographical model in which corner holes are considered to be the nuclei of the 7×7 domains (Miyake *et al*. 1997).

Experiments and Results

Flat N-type Si(111) samples (As-doped, resistance = 0.375–0.625 Ω cm) were cleaned ultrasonically for 10 min by acetone, prebaked for 10 h, followed by flashing to 1250˚C, and cooled down to room temperature. The flashing temperature and the direction of the current flow were such that step bunching occurred (Latyshev *et al*. 1989). Scanning tunneling microscopy observation confirmed the formation of step bunching as well as the fact that the surface is completely covered with the 7×7 reconstruction. This substrate was flashed again at 1250˚C and was quenched by turning off the power supply.

The inset in Figure 1 shows a typical STM image of the surface of a quenched Si(111) surface.The small triangles observed in the inset, which has six adatoms each, are the half unit of the 7×7 reconstruction. These half units form a triangle-shaped 7×7 domain. Many 7×7 domains are observed surrounded by the disordered 1×1 areas. Even though many small 2×4, 2×2, and 2×8 phases are observed in the disordered region, the atomic structures of the disordered area remain unclear. They have a strong tendency to appear bright and like a single or a cluster of adatoms in the filled state STM images, although they appear dark in the

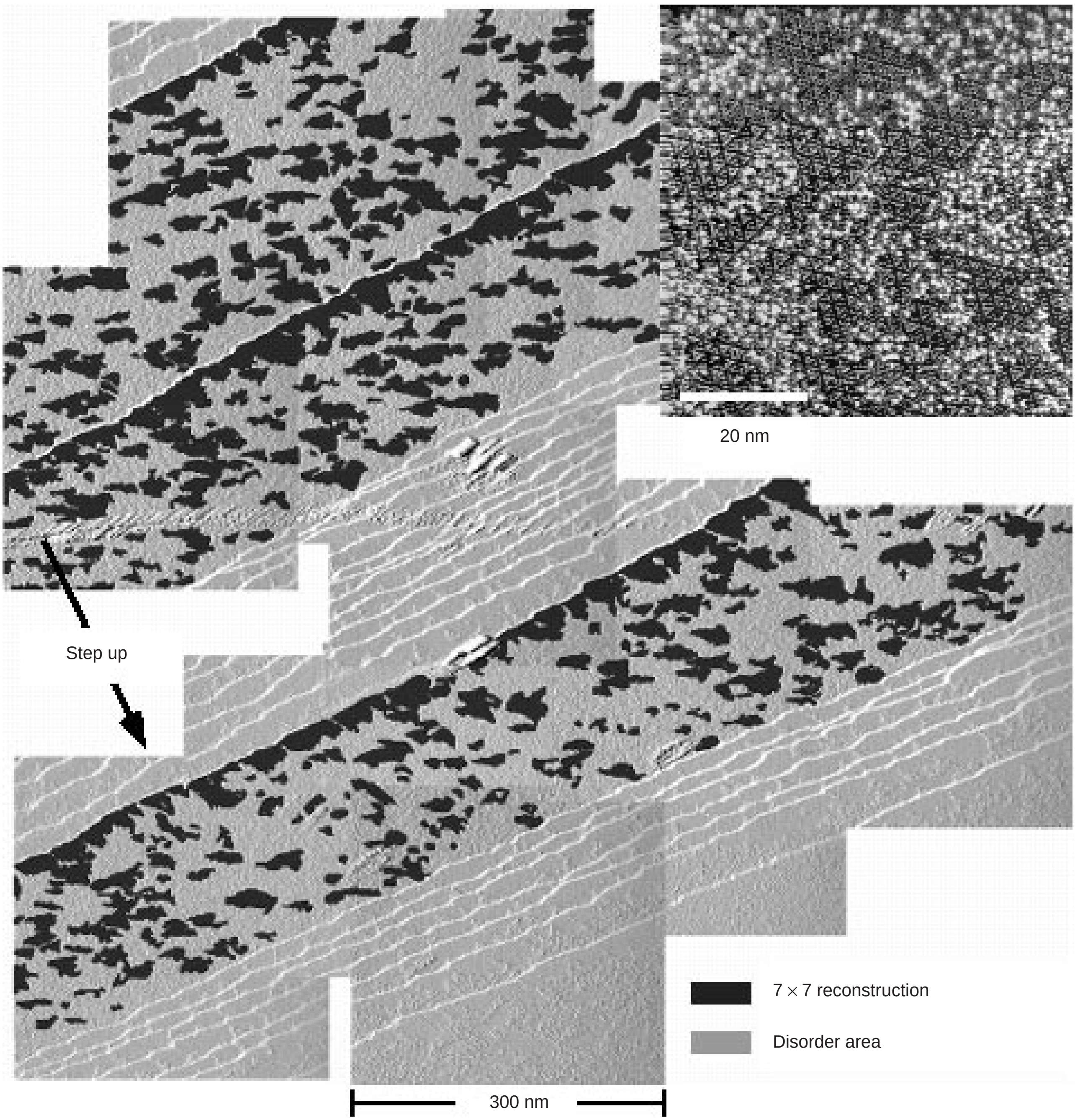

FIG. 1 Set of combined scanning tunneling microscopy images showing a wide region of the quenched surface. Step bunching has formed and the terrace widths exceed 200 nm. The black regions are reconstructed to 7×7. The inset shows a close-up of the quenched surface. Tunneling voltage –1V, current 0.3 nA. The triangle-shaped regions are reconstructed to 7×7.

empty state STM images (Miyake 1995, Miyake *et al*. 1995). This aspect has many implications concerning the formation process of the 7×7 domain. It is natural to assume that each 7×7 domain has grown out from a nucleate core (Miyake 1995). The latest studies report that the nucleation of a corner hole is the rate-limiting process for the formation of the 7×7 structure (Miyake 1998). This implies that the key process for the development of the 7×7 domains is the formation of an isolated single corner hole in the disordered region and that the 7×7 domain grows centering the corner hole. This point is a basic assumption we employ hereafter regarding the formation process of the 7×7 domains.

A wide region of the surface observed by STM is shown in Figure 1. The dark and light gray regions represent the 7×7 and disordered regions, respectively. All of the steps observed were misoriented in the $\langle 11\bar{2} \rangle$ direction. At the first look at Figure 1, it is clear that step bunching has occurred on the surface, and wide terraces exceeding 200 nm in width are observed. Also, an intense increase in the existence probability of the 7×7 reconstruction at the upper step site is clearly notable. From Figure 1, the existence probabilities of the 7×7 structure versus the distance from the upper and down step edge were measured, as shown in Figure 2. As reported before, the upper step edge shows a high existence probability that gradually decreases to a constant value (the existence probability of the terrace) as the distance from the upper step edge increases (Tokumoto and Iwatsukui 1993). On the other hand, we observed a considerable decrease in the existence probability of the 7×7 reconstruction at the down step edge. The existence probability gradually increases to a constant value as the distance from the lower step edge increases. Since the existence probabilities from the upper and down step edge recover to the same constant value, which is the existence probability of the 7×7 reconstruction on the terrace, we can conclude that the decrease in this existence probability at the down step edge is not influenced by the upper step edge bounding the other side of the terrace and reflects the characteristics of the down step edge.

Discussion

Several factors can be considered to be the origin of the observed decrease in the existence probability. First we consider whether or not the electromigration phenomena (Yasunaga 1991) and the step motion caused by the difference in adatom density between the 7×7 reconstruction and disordered 1×1 phase can explain the observed decrease in probability. It is known that the disordered phase has a higher density of adatoms compared with the 7×7 phase (Yang and Williams 1994). Therefore, we assume that areas covered with high density of adatoms will have a high probability to remain as disordered during the quenching process. Disordered areas can be regarded as regions where the superabundant adatoms created during the formation of the 7×7 phases were dumped.

Fluctuation of steps caused by fluctuation between the number of adatoms incorporating into and detaching from the step edge might be the origin of the observed decrease in the probability of 7×7 near the down step edges. Such step fluctuations have been directly observed by in situ high temperature STM experiments (Tokumoto *et al*. 1992). If the fluctuation is large, then the down step sites will have a small chance to form the 7×7 reconstruction. This is because when steps recede as a result of fluctuation, the newly exposed regions at the down step edge have a lower possibility to form a growth nucleus and growth in the 7×7 domain, in this case 20 nm: the distance the down step edge influences the existence probability of the 7×7 phase and represents the char-

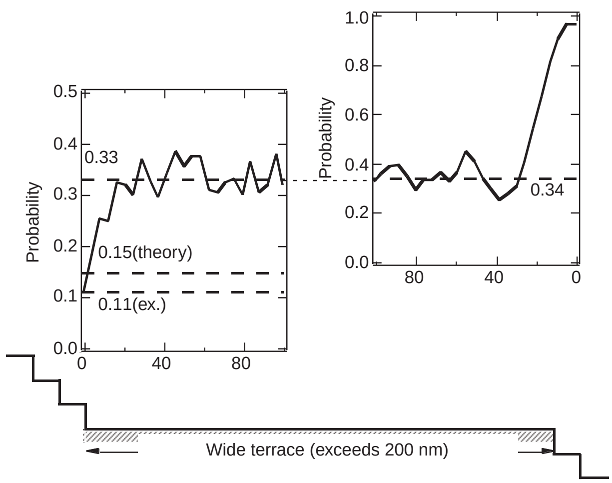

FIG. 2 The existence probability of the 7×7 reconstruction from the up (right) and down (left) step edge versus distance calculated from the scanning tunneling microscopy image of Figure 2. The averaged existence probability on the terrace is 0.34 and 0.33 (the regions which are influenced by the step edges were excluded in the averaging).

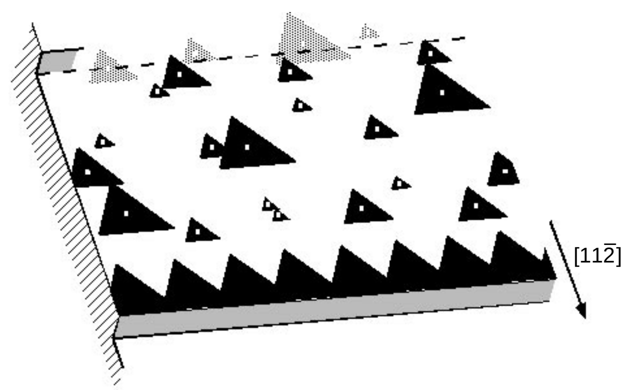

FIG. 3 Schematic showing how the down step edge influences the total area of the 7×7 domains. The black-triangles represent the 7×7 domains. The white dot in the center is the growth nucleus of the domain. Light gray triangles are 7×7 domains which would exist if the step did not exist, but do not when the step exists.

acteristic length of the fluctuation of the steps at the temperature where the kinetics of steps movement were frozen. A similar explanation applies when the steps recede as a result of sublimation, even though sublimation is negligible at the temperatures at which the 7×7 structure forms. As mentioned above, the disordered 1×1 phase has a higher density of adatoms than the 7×7 phase (Yang and Williams 1994). This means that as the total area of 7×7 increases, increasingly more excess adatoms come into being on the surface. Steps will serve as sites to absorb these excess adatoms and consequently they will move forward. In such a situation, the above discussion is not valid because steps do not recede.

Electromigration is a phenomenon in which an electrical current applied to the sample exerts a force on the surface adatoms to migrate (Yasunaga 1991). This phenomenon is the direct origin of the step bunching phenomenon utilized to fabricate the wide terraces in this study (Latyshev *et al*. 1989). Recently it was elucidated that Si adatoms on the surface are positively charged and migrate toward the direction of the electrical current flow (Hibino *et al*. 1996). It is possible that surface adatoms diffuse across the terrace by electromigration and accumulate at the down step edges, because they feel that a large activation energy diffuses over the step edge or is incorporated into the step edges (Schwoebel and Shipsey 1966). An accumulation of adatoms at down step edges will give a lower 7×7 existence probability. However, during quenching, no direct current is applied to the substrate. The power supply is cut off at 1250˚C and 7×7 forms only when the surface has cooled down below the 7×7–1×1 phase transition temperature around 840˚C; thus, there exists no electric field when the 7×7 reconstruction forms on the surface, and we exclude electromigration as the cause of the decrease in existence probability of the 7×7 reconstruction.

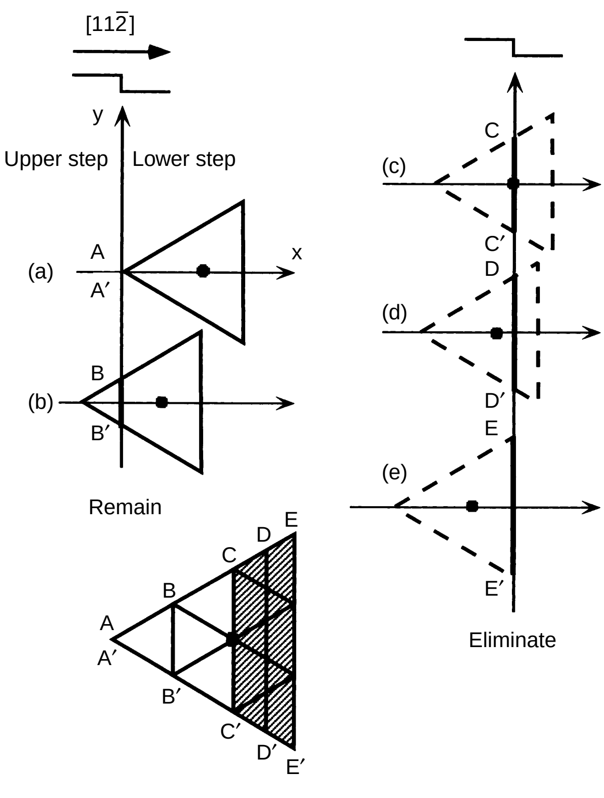

FIG. 4 Series of schematic displayed to visualize the procedure to estimate the existence probability of the 7×7 domains at the down step edge. See text for details.

Another simple model is proposed by which it is possible to explain the decrease in existence probability of the 7×7 reconstruction. The model assumes corner holes as growth nuclei of the 7×7 domain (Miyake 1998, Miyake *et al*. 1997) as schematically shown in Figure 3. Within the frame of this model, the existence probability of the 7×7 domain must definitely decrease near the down step sites. This is because sites close to the down step edge have a small number of nuclei in the vicinity when compared with sites on the terrace. While sites on the terrace are surrounded by nuclei in every direction, those nearby the down step edges lack the nuclei beyond the down step edge. This aspect is shown in Figure 3. In this schematic, the black triangles represent the 7×7 domains and the white spot in the center of each domain the nuclei. As the steps are misoriented in the <11 $\bar{2}$> direction, the triangle-shaped 7×7 domains are positioned so that one of the sides of the triangles is parallel to the step edge. The light gray triangles are the 7×7 domains which exist if the down step edge did not exist, although these 7×7 domains do not exist when the step exists. The down step edge would experience a lower existence probability of the 7×7 reconstruction than the terrace because of this elimination. The average domain width was 25 nm and this is consistent with 20 nm: the distance the down step edges influence the existence probability of the 7×7 reconstruction. We can easily estimate the existence probability (compared with the terrace) exactly at the down step edge predicted by this model, as shown in Figure 4. Consider a plane. The y-axis represents an imaginary step edge and the positive x-region the terrace. The ratio of decrease of the 7×7 domain at the step edge can be estimated by locating a growth nucleus at the center of each 7×7 domain (same size) at every point on the x-axis and counting the total eliminated 7×7 area by the step edge against the remaining 7×7 area at the step edge. This counting process can be visualized by considering a triangle-shaped 7×7 domain with a growth nucleus at the center approaching the step edge from the infinite as displayed in Figure 4. Figure 4 (a) and (b) shows cases in which the 7×7 domain remains while Figure 4 (c), (d), and (e) shows cases in which the domains are eliminated by the step. Each contribution to the area (eliminated or remaining) is different, as marked in each figure as AA′–EE′. These contributions are transformed into another triangle, as displayed in Figure 4 (f). Now it is easy to understand that the shaded regions are eliminated and the white area remains. Thus, at the down step edge, our model predicts that the 7×7 existence probability is 4/9 of that of the terrace (0.33), which gives 0.11. The actual existence probability was 0.15.

The small deviation between the model and experiment can be attributed to many factors. It is possible that a distortion in structure at the down step edge suppresses the formation of the growth nucleus, or the growth rate of the 7×7 domain is slow compared with that of the terrace because of the presence of an elastic strain field induced by the down step edge, and the critical size of the 7×7 domain is larger compared with that of the terrace.

Conclusion

We have fabricated a surface with wide terraces by utilizing the step bunching phenomenon to study the effect of the down step edges on the formation of the 7×7 reconstruction. The surface with wide terraces was quenched through the 1×1–7×7 phase transition, freezing the formation process of the 7×7 reconstruction. At the down step edge we observed a considerable decrease in the existence probability. This decrease cannot be explained by electromigration and by steps advancement caused by the difference in adatom density between the 7×7 and disordered structure. We show that a simple topographic model, considering a corner hole as a growth nucleus of the 7×7 domain, explains the prime characteristics of the observed decrease in probability.

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