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# Self-Organized Nanostructure Formation on High-Index Si Surfaces Induced by Ga

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It had been reported that 1 ML Ga deposition on Si(113) surface changes the flat (113) surface to nano-facet structure of (112) and (115) surfaces. In this work, details of the self-organized nano-faceting process on Si(113) surface induced by Ga deposition has been investigated using an scanning tunneling microscopy. The faceting process at 800 K Ga deposition is as follows: Initially, 2-dimensional (2D) triangular island formation occurred followed by 2D to 3D island transformation at 0.6 ML of Ga coverage. For further deposition, the surface changes into single width (112)/(115) pair structure. Finally, both of (112) and (115) 'facets' bunch up respectively and (112)/(115) nanofacet structure is formed. It is clarified that the nanofacet length along to $[1\bar{1}0]$ direction was limited by the 3D island distribution. It is also found that low temperature Ga deposition followed by high temperature annealing can suppress 3D island formation and well-ordered nanofacet structure is successfully obtained.

Key words: Si(113), Ga, nanofacet

## 1 INTRODUCTION

It is well known that Si(113) surface is atomically flat and its surface reconstruction is 3×2[1, 2]. However, foreign material deposition on Si(113) causes the flat surface to facet structure[3–8]. It has been reported that Au deposition of flat (113) surface leads to facet structure that consists of (113), (119) and (225) surfaces[5]. There are also several reports on Ga deposition on high-index Si surfaces[3, 4, 7, 8]. Baski *et al.*[3] reported that Ga deposition on faceted Si(112) surface changed the faceted surface into flat (112) with $N\times1$ ($N$=4~8) reconstruction. In the previous work[7, 8], we have been reported that 1 ML Ga deposition at about 870 K makes one dimensional nano facet structure of (112) and (115). The (112) surface had $N\times1$ reconstruction and the other had 4×1. This self-organized nano-faceting occurred relatively low temperature as compared with Si surface diffusion (such as step bunching *etc.*), therefore Ga induced faceting process is interesting from view points of surface diffusion and mass transport. The width of both (112) and (115) facets are about 5 nm, therefore it is expected that the surface can be used as quantum devices or a template of quantum device fabrication. It is also expected that it can be useful for a substrate of functional organic film growth.

In this study, details of surface morphology change of Ga adsorbed Si(113) surfaces has been investigated using an scanning tunneling microscopy (STM) to clarify facet formation mechanism and to find a key to control the facet structure.

## 2 EXPERIMENTAL

Si(113) substrate used was n-type with resistivity of 2.4~4.2 Ω·cm. The substrate was cleaned by SEMICOCLEAN23 (Furuuchi Chemical Corp.), distilled water and acetone in an ultrasonic cleaner. Subsequently, it was annealed at 770 K for 10~20 hours, followed by flash heating at about 1520 K for few seconds in an ultra-high vacuum (UHV) camber. Thus, atomically flat clean Si(113)3×2 surface was obtained. As reported in the previous paper[7], the initial surface has atomic steps in every ~200 nm and the atomic steps are almost straight. Substrates were heated by direct current, and the temperature was measured by an IR thermometer. The STM apparatus used is commercial high-temperature STM (JSTM-4500VT, JEOL Inc.) with a reflection high-energy electron diffraction (RHEED). Ga was evaporated from $Al_2O_3$ coated W basket. Ga evaporation rate was about 0.10 ML/min that was estimated from a coverage at which Ga/Si(111)$\sqrt{3}\times\sqrt{3}$ structure appears[9]. Base pressure of the UHV chamber was $2\times10^{-8}$ Pa, and pressure during Ga deposition was below $2\times10^{-7}$ Pa. All STM images were observed at room temperature to prevent thermal morphological change during the observations.

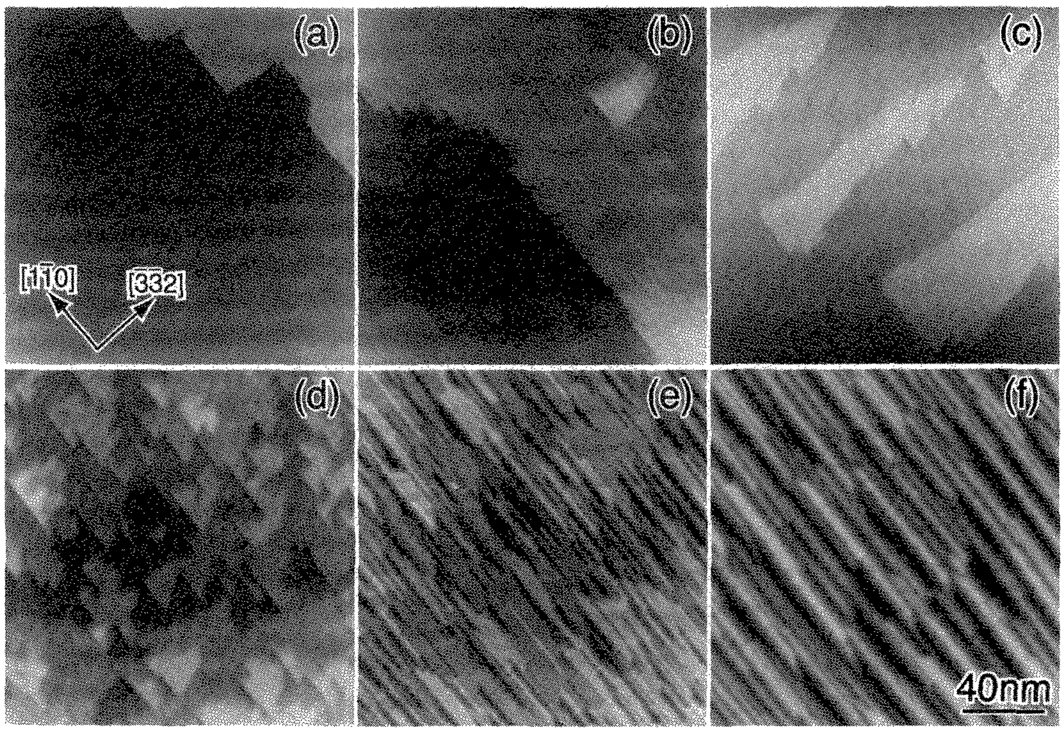

Fig. 1: STM images of Ga deposited Si(113) surface at 800 K. Respective Ga coverage are (a) 0.3 ML, (b) 0.4 ML, (c) 0.5 ML, (d) 0.6 ML, (e) 0.7 ML and (f) 1.0 ML. Sample bias voltage and tunneling current used were 1.6 V and 0.3 nA. All images are taken at room temperature.

## 3 RESULTS AND DISCUSSION

Fig. 1 shows Ga deposition process at substrate temperature of 800 K. As already reported[7], surface reconstruction changes from 3×2 to 3×1 at about 0.1 ML of Ga deposition (no corresponding image is shown here). At 0.3 ML of Ga deposition (Fig. 1(a)), atomic steps, which had been almost straight along to [1$\bar{1}$0] direction, became zigzag shape as shown in the figure. It seems that [$\bar{1}$10] steps became preferable than [33$\bar{2}$] steps. At 0.4 ML (Fig. 1(b)), a triangular 2-dimensional (2D) island nucleated on a terrace. Most of the nucleation sites of 2D islands were about 50 nm apart from neighboring steps. In addition, 2×2 surface reconstruction grew from an atomic step to both upper and lower sides of the step. At this coverage, 2×2 area expanded to 30~50 nm from a step. Therefore it is considered that excess Si atoms, which were supplied by 3×1 to 2×2 structural change, diffused on the surface and stick to atomic steps to grow the steps and also created 2D nuclei at 3×1/2×2 boundary.

The next stage is 2D island growth toward [$\bar{3}\bar{3}$2] direction (Fig. 1(c)). As a result, 2D island shape changed to elongated triangle. This also suggests that [$\bar{1}$10] step energy is lower than that of [33$\bar{2}$] step. At this coverage (0.5 ML), whole part of the surface, including the 2D islands, changed to 2×2 reconstruction. At 0.6 ML (Fig. 1(d)), 3D growth started and surface morphology drastically changed from the previous coverage. The elongated triangular islands disappeared and regular triangular island reappeared. It seems that Si atoms in the 2D islands were detached and also Si atoms in the base layer moved up. Most of the islands have 2~3 layers height and [33$\bar{2}$] edges of the islands tends to overlap. An expanded image of the Fig. 1(d) is shown in Fig. 2 (differential image is used to emphasize surface reconstruction). As indicated by arrows in the figure, (112) facets were formed at [33$\bar{2}$] step edges and surface reconstruction on (112) facets were $N\times1$ ($N$=4~8)[3, 7]. It is suggested that surface free energy of the (112)$N\times1$ structure is lower than that of (113)2×2 structure at more than 0.5 ML Ga coverage.

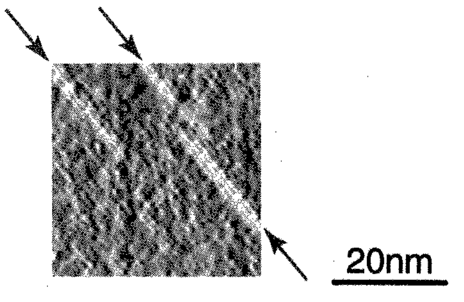

Fig. 2: Differential current image of Si(113) surface with Ga coverage of 0.6 ML. (112)$N\times1$ ($N$=4~8) facets are indicated by arrows. The other part of the surface is 2×2 structure.

For further deposition of Ga, the triangular islands grew toward [1$\bar{1}$0] direction to expand the

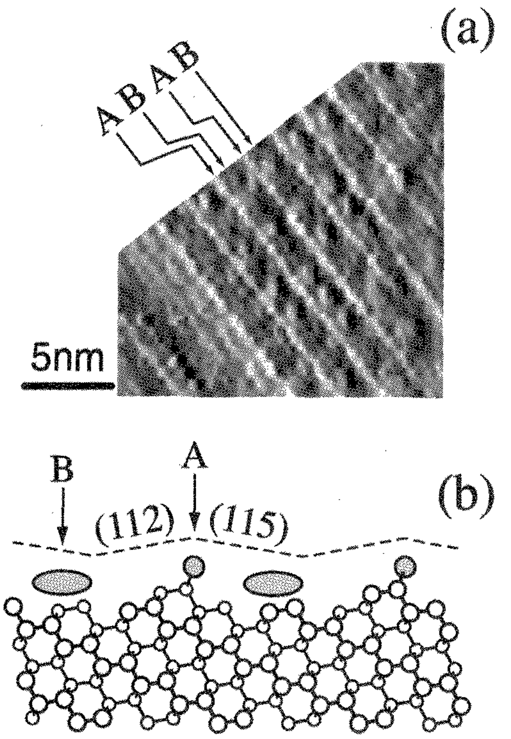

Fig. 3: (a) Differential current image of Si(113) surface with Ga coverage of 0.7 ML. (b) Cross sectional illustration of terrace area of the above image. Open circles and gray circles indicate Si and Ga atoms respectively. Gray ellipsoids indicate bright position in the STM image, which correspond to protrusions in empty state image. Corresponding positions between figures (a) and (b) are indicated as 'A' and 'B'.

(112) area and the surface structure of the terrace area became as shown in Fig 3(a). It is observed in the STM image that a unit of (112)$N\times 1$('A' in the figure) and (115)$4\times 1$[7]('B' in the figure) laid alternately. Thus, it is considered that terrace area of Fig. 1(e) consists of single width (112) and (115) 'facets' pairs as shown in Fig 3(b). A structural model for Ga/Si(112)$N\times 1$ structure proposed by Baski *et al.*[10] is used in the figure. For (115) facet, bright contrast position (*i.e.* protrusion in empty state image) is shown in the model, however details of atomic positions has not been decided yet. Finally, both of (112) and (115) 'facets' bunched up respectively and (112)/(115) nanofacet structure was formed (Fig. 1(f)). An average facet length along to $[1\bar{1}0]$ direction was about 50 nm. It is considered that the length was mainly limited by 3D islands at 0.7 ML (Fig. 1(e)).

If it is possible to suppress 3D island formation, it is expected to fabricate longer nanofacets. It is considered that reduction of mass transportation is essential to suppress 3D island formation, therefore low temperature Ga deposition was carried out. 1.3 ML Ga was deposited on Si(113) surface at 660 K followed by an annealing at 800 K. Surface morphology change during the annealing process is shown in Fig. 4. As deposited (Fig. 4(a)), the surface was relatively flat as compared with 800 K case (Fig. 1(f)). It is considered that short diffusion length suppress mass transport for facet structure formation. The surface structure is single width (112)/(115) pairs which is similar to that of 0.7 ML coverage at 800 K (Fig. 1(e)) but few multiple height islands were observed.

After annealing the surface at 800 K for 30~60 min (Fig. 4(b) and (c)), double width (112)/(115) pairs were formed and grew toward $[1\bar{1}0]$ direction. As a result, well-ordered 1D like facet structure was obtained as shown in Fig. 4(c). Most of the nanofacet width corresponds to 2 units (1.9 nm) and the length along to $[1\bar{1}0]$ direction is more than 100 nm. For 120 min of annealing (Fig. 4(d)), a deep groove start to appear as shown by a white ellipsoid. At the same time, (115)$4\times 1$ structure started to disappear around the groove structure. While on the (112) facets, $N\times 1$ reconstruction remained. In the previous work[7], it has been estimated that Ga coverage on the (115)$4\times 1$ structure is 0.8 ML. In addition, it is well known that Ga easily desorbs from Si surfaces at around 900 K. Therefore it is considered that Ga started to reevaporate from (115) facets and the (115) facets became unstable. For further annealing, the groove area increased and surface roughness increased with annealing time as shown in Fig. 4(e) and (f). As described above, well-ordered 1D nanofacets was obtained by Ga deposition at 660 K followed by an annealing at 800 K for 60 min. However, over-annealing caused Ga desorption and the quality of 1D nanofacet structure deteriorated.

## 4 SUMMARY

Details of self-organized nano-faceting process on Si(113) surface induced by Ga deposition has been investigated by STM. The faceting process at 800 K deposition was as follows: Initially, excess Si atoms, which are supplied by $3\times 1$ to $2\times 2$ reconstruction, form 2-dimensional (2D) triangular islands. At 0.6 ML of Ga deposition, 2D islands are restructured into 3D island with small (112) facets on $[33\bar{2}]$ step edges. For further deposition of Ga, the surface changes into single width (112)/(115) pair structure. Finally, both of (112) and (115) 'facets' bunch up respectively and (112)/(115) nanofacet structure is formed. It was clarified that the nanofacet length along to $[1\bar{1}0]$ direction was limited by the 3D island distribution. It was also found that low temperature (660 K) Ga deposition followed by high temperature (800 K) annealing can suppress the 3D island formation and well-ordered nanofacet structure with length more than 100 nm was successfully obtained. However, over-annealing of the surface resulted in Ga desorption from (115) facets and the nanofacet structure was destroyed.

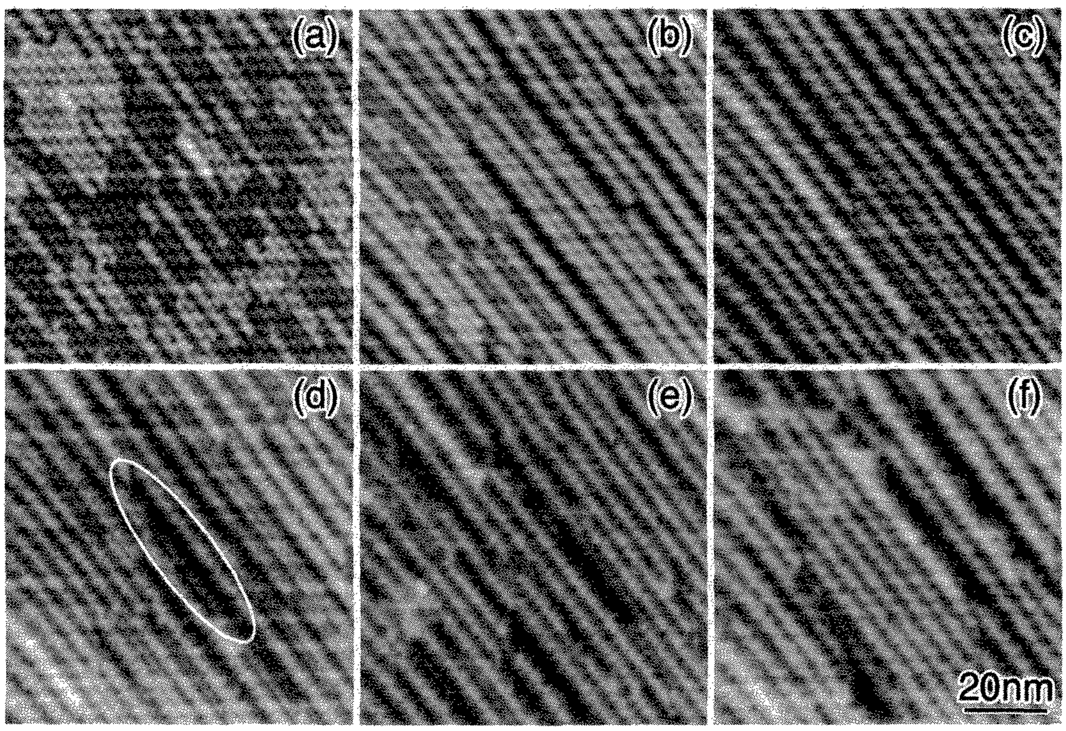

Fig. 4: Annealing process of Si(113) surface with 1.3 ML of Ga. (a) as deposited at 660 K, (b)-(f) after annealed at 800 K for 30 min, 60 min, 120 min, 180 min and 240 min respectively. All images are taken at room temperature. Substrate direction is the same as Fig. 1.

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