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Ga-induced restructuring of Si(112) and Si(337)

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The adsorption of gallium on Si(112) and Si(337) has been studied with scanning tunneling microscopy. When clean, these two high-index surfaces are unstable and facet to other orientations: (112) to (111)- and (337)-like nanofacets, and (337) to the stable (5 5 12) plane. When Ga is adsorbed onto each of these surfaces and annealed, the top surface layers undergo substantial rearrangements, exposing Ga-reconstructed (112) planes in both cases. © *1996 American Vacuum Society.*

I. INTRODUCTION

Several approaches have been explored to tailor the surface morphology and growth behavior of semiconductor systems. One approach is to use a surfactant overlayer to alter the energetics and/or kinetics associated with the growth front. For example, adsorbates such as Ga and Sb have been investigated as surfactants to improve the homoepitaxial growth of Si and heteroepitaxial growth of Si–Ge systems.[1,2] Another approach is to initiate growth on a high-index substrate. Such substrates are expected to have a higher density of step edges than occur on their low-index counterparts, leading to enhanced step flow and presumably improved growth.[3] Our recent scanning tunneling microscopy (STM) studies of clean Si(112) and Si(337) surfaces, however, reveal that these particular high-index surfaces facet to other orientations: (112) reconstructs into quasiperiodic, sawtooth-like nanofacets composed of reconstructed (111)- and (337)-like planes,[4] whereas (337) facets to (5 5 12), a recently discovered stable orientation.[5,6] We have now investigated how Ga influences the morphology of these two high-index surfaces. In addition to its possible role as a growth surfactant, Ga is an important constituent of III–V and nitride-based semiconductor heterostructures.

II. EXPERIMENT

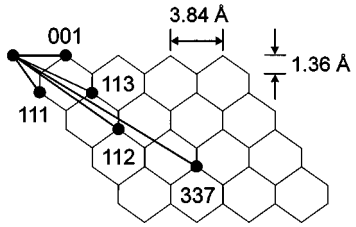
These experiments were performed in ultrahigh vacuum using Si wafers oriented to within 0.5° of (112) or (337). To obtain a clean surface, each sample was chemically precleaned, mounted onto a button heater in vacuum, degassed at 600 °C, and then flashed to ≈1150 °C for 60 s (pressure $\leqslant 2\times10^{-9}$ Torr). Gallium was deposited from a heated tungsten basket onto samples at temperatures below 150 °C. After depositing >1 monolayer of Ga, the surface was annealed to 500±50 °C for 10 min. On the Si(112) surface, this procedure resulted in a 6×1 low-energy electron-diffraction (LEED) pattern, thought to correspond to 5/6 Ga atoms per bulk-terminated (112) unit cell.[7] Auger electron spectroscopy (AES) measurements indicated a ratio of the Ga(55 eV) to Si(92 eV) signals of 0.04±0.005 on both the (112) and (337) surfaces, consistent with values found in the literature.[8] STM images of the filled and empty electronic states were acquired at room temperature with a constant current between 0.1 and 0.3 nA and bias voltages between 1.0 and 2.5 V.

III. DISCUSSION

The first of the two high-index surfaces investigated here, Si(112), is tilted 19.5° away from the (111) surface toward (001) [see Fig. 1]. The clean (112) surface undergoes a complex reconstruction involving the topmost ~7 layers.[4] The corrugated nature of this reconstruction is apparent in the STM image shown in Fig. 2(a). Each of the stripes oriented along the [1$\bar{1}$0] direction corresponds to a sawtooth-like nanofacet consisting of a short, unit-cell-wide reconstructed (111) plane (7×7 or 5×5) opposed by a longer 60–100-Å-wide (337)-like plane. On well-oriented samples these nanofacets may extend for microns along the [1$\bar{1}$0] direction. The creation of the nanofacets results from the lower surface energies associated with the reconstructed (111)- and (337)-like planes.[9]

When an overlayer of Ga is deposited onto the nanofaceted (112) surface and annealed, a large-scale rearrangement occurs: The nanofacets disappear and the surface returns to its basal (112) orientation. As shown in Fig. 2(b), the Ga-covered surface consists of highly anisotropic, (112)-oriented islands. These islands extend for microns along the [1$\bar{1}$0] direction but are less than 1000 Å wide. This anisotropy is attributed to the linear structure of the original nanofacets. Over a micron-square region, the height variation of this surface ranges from five to seven atomic layers, comparable to the height of a single nanofacet on the clean surface.

A higher-resolution, empty-state image of the Ga-terminated (112) surface is shown in Fig. 2(c). It reveals that the islands consist of periodic rows oriented along the [11$\bar{0}$] direction, which are interrupted by an array of [$\bar{1}$11]-oriented dark trenches. The period of the rows along [111] equals the length of the (112) unit cell, 9.4 Å, confirming the (112) orientation of the Ga-terminated islands. The dark trenches occur with spacings of 19–27 Å along [1$\bar{1}$0], corresponding to 6±1 times the bulk-terminated (112) unit-cell width. This structure accounts for the 6×1 LEED pattern previously reported for the Ga:Si(112) system.[7,8] It should be noted that filled-state images of this surface do not display the same prominent dark trenches shown here; rather, more subtle variations occur along the rows with the same periodicity. Dual-bias, atomic-resolution images of this surface and a proposed atomic model of the Ga:Si(112)6×1 reconstruction will be presented elsewhere.[10]



	(111)	(112)	(337)	(113)	(001)
Angle	0°	19.5°	23.5°	29.5°	54.7°
Length (Å)	3.33	9.41	15.7	6.37	3.84

FIG. 1. Side-view model of a Si crystal lattice bounded by the (111) and (001) planes. The intersections of the lattice lines represent projections of atomic positions onto the {110} plane (i.e., the plane of the page). On this lattice, a variety of orientations are indicated by line segments whose lengths equal one unit cell of the associated bulk-terminated surface. The table lists the angle with respect to (111) and the bulk-terminated unit-cell length (projected onto the {110} plane) for each orientation.

The second high-index surface investigated here, Si(337), is tilted 23.5° away from the (111) surface toward (001) [4° from (112); see Fig. 1]. Figure 3(a) displays an image of the clean (337) surface, composed of an array of relatively wide terraces. Our recent STM studies demonstrated that these terraces correspond to the stable Si(5 5 12):2×1 surface.[5] Because the (337) surface is oriented only ≈0.7° from (5 5 12), it forms relatively wide (5 5 12) terraces (500–1000 Å) separated by multiple-height steps or single unit-cell-wide 7×7 (or 5×5) reconstructed (111) planes. In general, it appears that clean Si surfaces oriented to within a few degrees of (5 5 12) facet to this orientation.[4–6]

After an overlayer of Ga is deposited onto the (337) surface and annealed, the initially terraced surface becomes noticeably corrugated, as shown in Fig. 3(b). These corrugations have a typical width of approximately 150 Å,[11] which is similar to the width of the nanofacets found on the clean (112) surface. In higher-resolution images [Fig. 3(c)], these corrugations are seen to arise from local faceting to two alternating planar orientations: (112) and (113). The (112) terraces are readily identified by their characteristic Ga-induced surface reconstruction [see Fig. 2(c) for reference]. The Ga:(113) terraces were identified by their angle with respect to the basal (337) plane and the size of the 3×2 reconstructed unit cells found in ordered regions (≈12 Å along [1̄10] by 13 Å along [332]). The assignment of the (113) orientation is also supported by the observation that approximately 50% more (112) than (113) is present on the surface, as required to maintain the basal orientation.

The surface morphological changes induced by Ga on the Si(112) and Si(337) are schematically illustrated in Fig. 4. After Ga adsorption, the initially nanofaceted Si(112) surface [Fig. 4(a)] planarizes to form (112)-oriented terraces [Fig. 4(b)], whereas the terraced Si(337) surface [Fig. 4(c)] breaks up into (112) and (113) nanofacets [Fig. 4(d)]. In both cases, Ga stabilizes the (112) surface orientation, an apparently low-energy configuration. It has recently been shown that Ga adsorption on Si(113) also causes faceting to Ga:Si(112).[12] In general, it appears that Ga-covered Si surfaces oriented between (112) and (113) facet to the Ga:(112)6×1 surface.

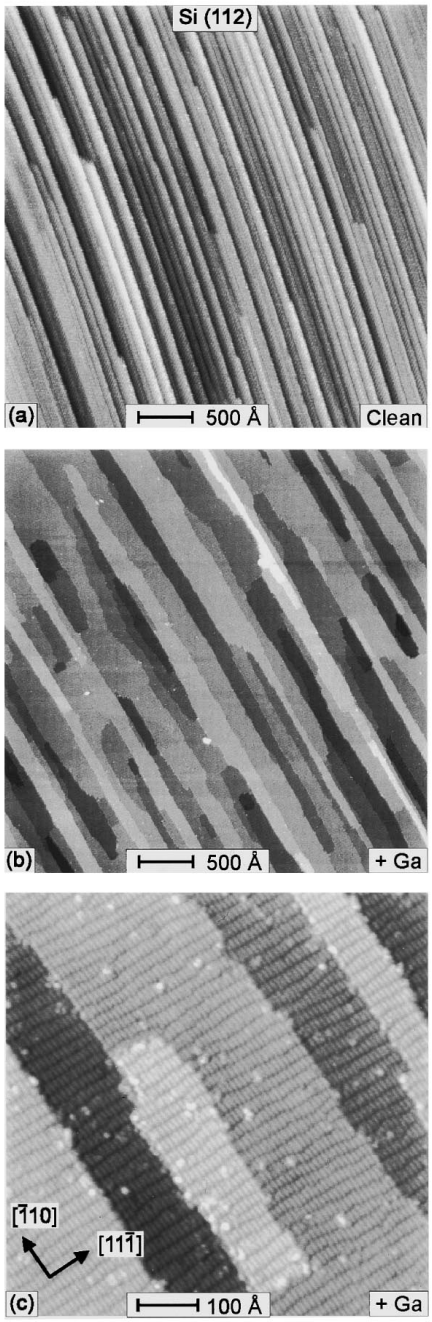


FIG. 2. (a) STM image of the clean Si(112) surface (4000×4000 Å^2). The striped corrugations are quasiperiodic, sawtooth-like nanofacets. (b) Image of the Ga:Si(112) surface (4000×4000 Å^2). The annealed Ga overlayer restores the surface to its basal (112) orientation. (c) Higher-resolution, empty-state image of the Ga-reconstructed (112) islands (700×700 Å^2, 2 V).

IV. CONCLUSION

The large-scale surface rearrangements induced by Ga on Si(112) and Si(337) are vivid examples of how an adsorbate can dramatically alter the energetics of a surface.[13] When Ga is adsorbed onto either of these high-index surfaces, it causes

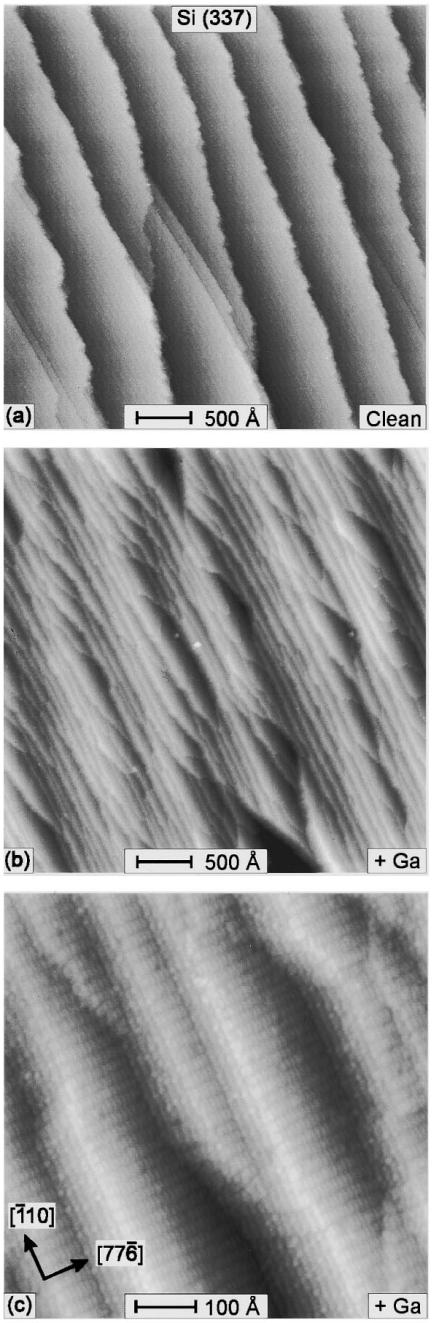


FIG. 3. (a) STM image of the clean Si(337) surface (4000×4000 Å^2). This surface facets to form large terraces with a (5 5 12) orientation. (b) Image of the Ga:Si(337) surface (4000×4000 Å^2). The annealed Ga overlayer causes the top surface layers to rearrange into a corrugated structure composed of alternating (112) and (113) planes. (c) Higher-resolution, empty-state image of the corrugated Ga:Si(337) surface (720×720 Å^2, 2 V).

a multilayer reconstruction in order to create Ga-reconstructed (112) planes. Whereas Si(5 5 12)2×1 is the lowest-energy structure for clean surfaces in the range of orientations studied here, Ga:Si(112)6×1 appears to be the stable structure for Ga-covered surfaces. This unexpected

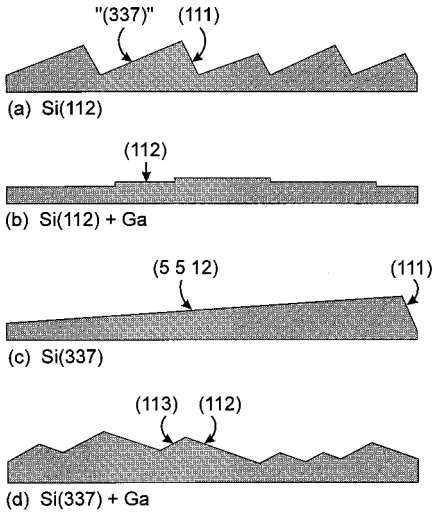


FIG. 4. Illustration of typical cross sections through a {110} plane of the clean and Ga-covered Si(112) and Si(337) surface structures. The vertical scale has been magnified five times with respect to the lateral scale, which spans approximately 600 Å. (a) Clean Si(112): sawtooth-like nanofacets composed of (337)-like and single unit-cell-wide (111)7×7 (or 5×5) planes; (b) Ga:Si(112): (112)-oriented terraces; (c) clean Si(337): large (5 5 12)2×1 terraces separated by steps or single unit-cell-wide reconstructed (111) planes; (d) Ga:Si(337): alternating (112)- and (113)-oriented terraces.

adsorbate-induced change in the stable surface structure demonstrates the difficulty in predicting the influence of surfactants and high-index substrates on heteroepitaxial growth.

ACKNOWLEDGMENTS

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