Si/Ge Growth on Stripe Patterned Si (001) Studied by Scanning Tunneling Microscopy

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Si and Ge growth on stripe patterned Si(001) substrates is studied using scanning tunneling microscopy. During Si buffer growth, the stripe morphology rapidly evolves to multifaceted "U" or "V" shaped forms due to transitions between different low energy {11n} side facets. Depending of the side wall geometry, subsequent Ge islands nucleate either on the side walls or in the center of stripes. Thus, the control of pattern topography is crucial for effective control of the nucleation sites.

Introduction

Self-organized Stranski-Krastanow island growth on pre-patterned substrates has attracted tremendous interest because it provides a route for controlled positioning of quantum dots in nano-electronic devices as well as for realization of quantum dot arrays [1] – [4]. Site controlled growth requires a tight control over the pattern morphology and growth conditions [1] – [5] and to obtain quantum dots with excellent electronic properties, sufficiently thick buffer layers have to be deposited to remove the defects induced by the patterning process [2], [3]. Therefore, a detailed understanding of the surface evolution and dot nucleation is crucial for control of the self-organization process. Here, in situ scanning tunneling microscopy is employed to study Si/Ge growth on a stripe-patterned Si (001) substrate. It is shown that a characteristic morphological transition from multifaceted "U" to "V" shaped grooves occurs during buffer growth and that a well-defined alignment of Ge islands only occurs for "V" shaped grooves.

Experimental

The investigations were carried out in a multi-chamber Si/Ge molecular beam epitaxy and scanning tunneling microscopy (STM) system. Stripe patterned Si (001) substrates were prepared by electron beam lithography and CF_4 reactive ion etching. The stripes with an etch depth of 35 nm and 350 nm period were aligned along the [110] surface direction. By varying the exposure dose, different groove widths from w = 70 to 280 nm were obtained, corresponding to pattern filling factors (ratio of w to the 350 nm period) of δ = 0.2 to 0.8. After cleaning and HF dipping for oxide removal, the samples were introduced into the vacuum system and shortly annealed at 740 °C. Si and Ge growth were performed at substrate temperatures between 450 to 600 °C and growth rates of ~3 and ~1 Å/min. STM images were recorded after different stages of growth after rapid cooling to room temperature to preserve the epitaxial surface structure.

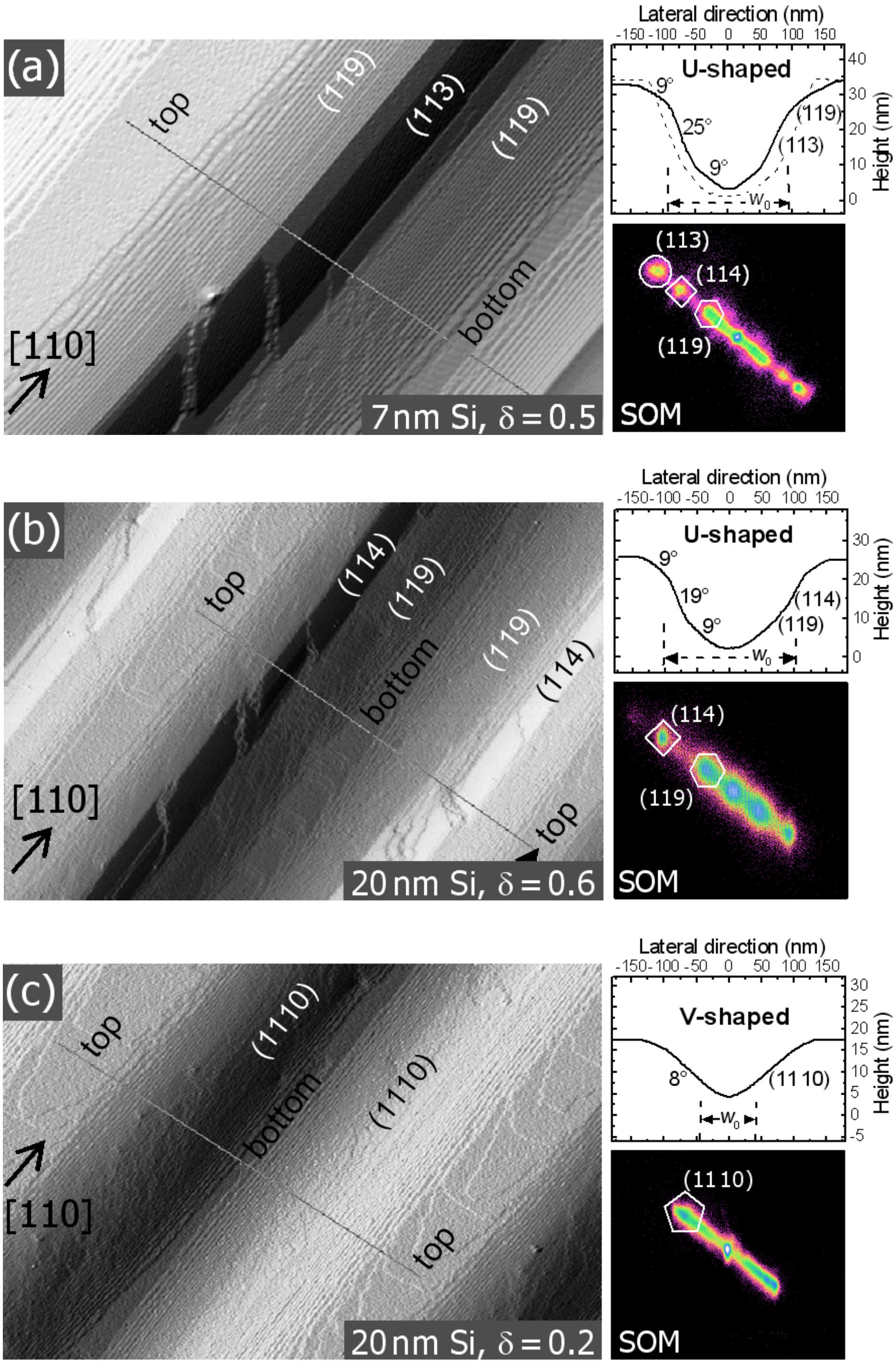

Fig. 1: STM images of stripe patterned Si (001) substrates after 520°C Si buffer growth: (a) “U” shaped grooves with {113} facets formed after 7 nm Si growth on stripes with δ = 0.5, (b) “U” shaped grooves with {114} facets after 20 nm Si on stripes with δ = 0.6, (c) “V” shaped grooves with {11 10} facets after 20 nm Si on stripes with δ = 0.2. STM image lateral size: (a) 0.35 µm, (b) and (c) 0.5 µm. The line profiles across the stripes as well as surface orientation density maps (SOM) of the STM images are shown on the right hand side and in (a) the stripe cross-section after low temperature buffer growth is additionally shown as dashed line.

Results

Usual Si buffer growth at temperatures above 600 °C leads to a complete pattern erasure within deposition of a few nm Si. Therefore, a two-step buffer growth was employed. First, 35 nm Si was deposited at a temperature of 450 °C to bury the residual carbon impurities on the surface. This leads to a rounding of the bottom of the grooves but their depth remains nearly unchanged. This was followed by Si growth at 520 °C for smoothening of the surface and further elimination of process defects. During the second buffer growth step the surface morphology rapidly evolves due to enhanced surface diffusion. This is illustrated by the sequence of STM images displayed in Fig. 1.

Already after 7 nm Si growth, the stripes assume a well defined multi facetted "U" shape as demonstrated by the STM image of Fig. 1 (a) for stripes with $\delta = 0.5$. From the cross-sectional profile analysis shown on the right hand side, there exist two short sidewall segments with ~9° inclination at the top and bottom of the grooves, and a steeper middle segment with ~25° inclination. The middle segment is therefore composed of {113} and {114} facets which pass over to {119} segments with small inclination towards the top and the bottom of the grooves. The corresponding surface orientation map (SOM) of the STM image exhibits two bright spots for the {113} and {114} facet orientations and a broader maximum at {119}. The high resolution STM image of the sidewall depicted in Fig. 2 (b), reveals that the {119} areas are composed of D_B type double steps, indicating that this surface part resembles a vicinal (001) surface. On the contrary, the steeper side wall areas appear completely flat and step free in the STM image and display the characteristic atomic structure of {113} and {114} Si surfaces [6].

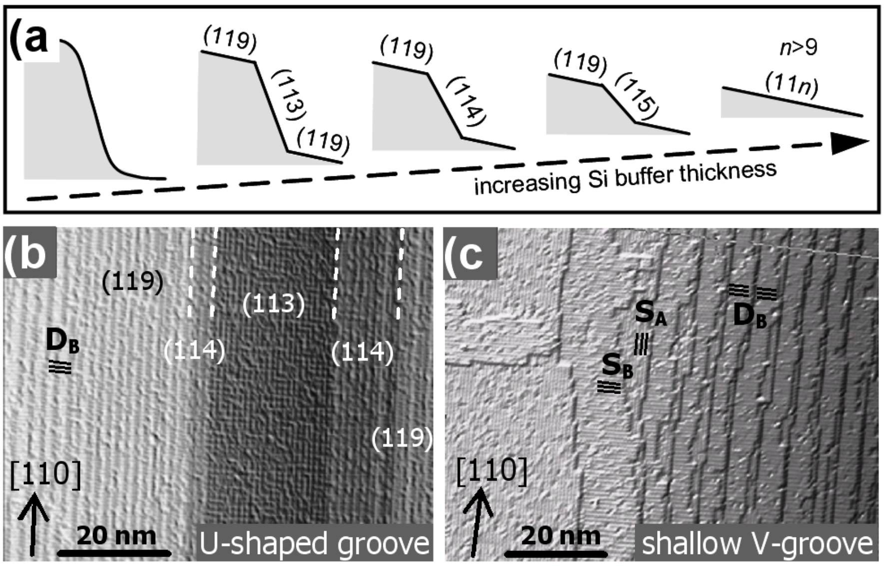

Fig. 2: (a) Schematic illustration of the evolution of the side wall profiles (b) High resolution STM image of the side wall of the multifaceted "U" groove shown in Fig. 1 (a) after 7 nm Si buffer growth. (c) STM image of a shallow "V" groove with about 4° side wall inclination. The triple lines indicate the directions of the Si dimer rows.

Continuing the Si buffer growth leads to a rapid shrinking of the steep middle sidewall segments and an expansion of the shallower {119} segments. This is demonstrated by the STM image of Fig. 1 (b) obtained after 20 nm Si deposition. The line profile analysis identifies inclinations of ~9° at the upper and lower part of the groove and of ~19° for the middle segment. Thus, the {113} area has been completely transformed to a {114} facet. Accordingly, only the {114} and {119} spots appear in the SOM. With further increasing Si thickness the {114} segment continuously shrinks and is replaced by a shorter {115} segment, which eventually also disappears such that only one extended ~9° side wall surface remains. This is illustrated schematically in Fig. 2 (a). The speed of this transformation strongly depends on the width and depth of the grooves and is much faster for patterns with small filling factor δ. This is demonstrated in Fig. 1 (c) for a pattern with $\delta = 0.2$ where already after 20 nm Si the surface been completely transformed to "V" shaped stripes with ~8° side walls as is indicated by the profile of Fig. 1 (c). The corresponding SOM shows a strongly elongated maximum around the {11 10} surface orientation. Thus, the side wall does not correspond to a unique stable facet orientation [6]. During further Si deposition the sidewall angle rapidly shrinks and a planar surface is reformed after about 30 nm. The high resolution STM image of such a shallow "V" groove is shown in Figs. 2 (c), where the average side wall inclination is only around 4°. As indicated, the side wall exhibits a D_B stepped terrace structure formed by merging of S_A and S_B single steps in the transition region at the edges of the grooves. This indicates that this region represents a vicinal surface.

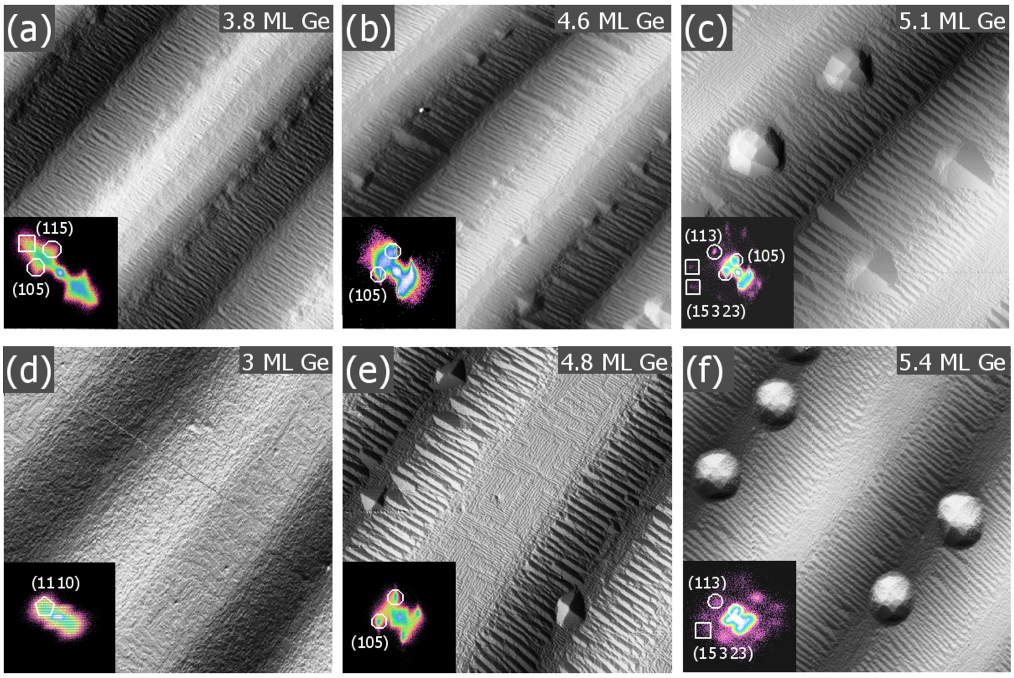

Fig. 3: STM images of Ge growth at 620 °C on stripe pattern Si surfaces after buffer growth. Top (a) – (c): Growth on "U" grooves with {119} and {115} sidewall facets and Ge thickness increasing from 3.8, 4.6 to 5.1 ML, respectively. Bottom (d) – (f): Growth on "V" grooves with {11 10} side faces and Ge thickness from 3, 4.8 to 5.4 ML, respectively. Ge first induces a {105} sidewall ripple structure and at higher coverages, pyramids and domes with characteristic {113} and {15 3 23} facets are formed, as indicated by the surface orientation maps (SOMs) depicted as insets. Image size: 0.5 × 0.5 μm^2.

To study the influence of the Si surface geometry on subsequent Ge island nucleation, Ge was deposited at 600 °C after buffer growth. The results for "U" shaped stripes with {115} sidewall segments are shown in Fig. 3 (a) – (c). During wetting layer growth, a distinct side wall ripple structure develops perpendicular to the stripes (Fig. 3 (a) after 3.8 ML Ge). The appearance of {105} spots in the SOM, indicates that these ripples consists of alternating {105} Ge micro-facets. On the steeper {115} side wall areas, no ripples but mounds with a few Å height are created, representing precursors for Ge island formation. Adding 0.8 ML Ge induces their transformation to {105} facetted Ge pyramids as demonstrated by the STM image of Fig. 3 (b). Further Ge deposition leads to an increasing island size and transformation to dome islands with characteristic {113} and {15 3 23} facets as shown by Fig. 3 (c) after 5.1 ML Ge. Evidently, all Ge islands in the “U” grooves are located in middle of the side walls.

STM images of Ge growth on “V” shaped stripes are presented in Fig. 3 (d) – (f). At 3 ML coverage (Fig. 3 (d)), the Ge wetting layer shows the typical (2×8) surface reconstruction of {001} Ge surfaces. After 4.8 ML Ge deposition (Fig. 3 (e)) pronounced side wall ripples appear again, but now they extend all the way from the top to the bottom of the grooves. At 4.8ML also the first {105} Ge pyramids appear, but they nucleate at the bottom of the grooves. This is because downward diffusion of Ge adatoms is not hindered by a steeper facet barrier. Upon further Ge deposition, the pyramids are transformed again to dome islands as shown by Fig. 3 (f). Accordingly, the characteristic {113} and {15 3 23} facet spots appear in the SOM. Nucleation of Ge dots at particular surface sites is driven by the variation of the chemical potential across the pattern structure due to variation of the local surface curvature. This generates an increased adatom flux towards the concave surface areas. For “V” grooves, the only concave area is at the bottom of the grooves, where material accumulation leads to a preferential Ge island formation. For “U” shaped grooves, concave surface parts also exist at the intersections between the {119} and steeper {114} or {115} side wall facets. Ge adatoms diffusing downward into the grooves accumulate at these intersections and thus, island formation sets in at the middle of the side walls.

Conclusion

In conclusion, Si growth on patterned substrate templates produces a characteristic morphology evolution from multifaceted “U” to “V” shaped geometries due to transitions between distinct side wall facets. Depending on the resulting surface morphology, subsequent Ge islands form either on the side walls or the center of the grooves. Multilayer Si/Ge growth drastically improves the control of the pattern morphology. Therefore, site-controlled Ge island nucleation is readily achieved by this growth sequence.

Acknowledgements

This work was supported by the Austrian Science Funds (SFB IR-ON).

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