Step-Bunching in Si with Faceted $Si_{0.55}Ge_{0.45}$ Top-Layers on High-Miscut Substrates

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We report on the influence of layer miscut on the step-bunching properties of the Si(001) surface. It is shown that for growth on substrates with a miscut of 4° along [110] the purely kinetic step-bunching instability is shifted to lower temperatures around 425 °C. Our epitaxial layers exhibit ripples with periods of ~90 nm and a height-modulation of more than 4 nm. Highly strained $Si_{0.55}Ge_{0.45}$ epilayers deposited on top of such rippled buffers decompose into faceted islands and additionally show preferential nucleation on the flanks of the step bunches in a narrow temperature range. Our experiments bridge the regimes of purely kinetic step-bunching and of strain-driven Stranski-Krastanov growth.

Introduction

The slightly miscut Si(001) surface is intrinsically unstable against kinetic-step-bunching. By using Si substrates with 4° miscut (along [110]) the period of the evolving ripple structure can be decreased to typically 90nm. p-modulation-doped layers on such substrates are expected to show pronounced interface roughness scattering in addition to alloy scattering. A variation of the interface roughness parameters should allow for a discrimination between these two mechanisms.

Experiments

We have reported, that the step-bunching instability is mainly influenced by the growth temperature [1], [2]. Concomitant with the decreasing period also the substrate temperature, where pronounced ripples are found, shifts to lower values. At Si growth rates of 0.2 Å/s a ripple pattern with few defects develops within a small temperature window around 425 °C. At slightly lower temperatures many defects are incorporated and the ripples decompose into islands, which are aligned in chains (Fig. 1, 400 °C).

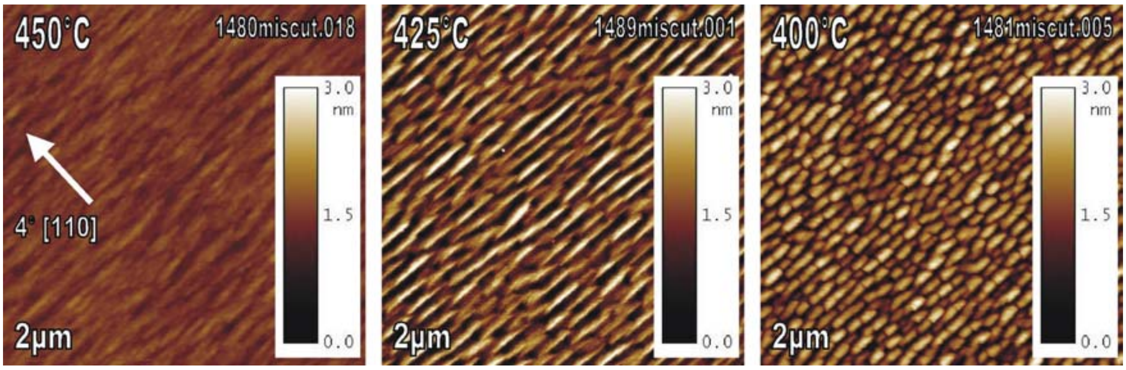

Fig. 1: AFM-images showing the substrate temperature dependence of step-bunching. The series of 500 Å thick Si-buffers grown on 4° [110] miscut samples (at 0.2 Å/s Si) proves that only within a small temperature range around 425 °C a pronounced ripple-structure is found.

For marginally higher temperatures the ripple structure fades away (Fig. 1, 450 °C).

Not only the influence of temperature was investigated, also a series of different Si-buffer layers was grown (Fig. 2). In the early stage of step-bunching (Fig. 2, 250 Å) there are many uncorrelated localized step-bunches. With increasing layer-thickness (500 Å) the individual bunch-segments merge and form well pronounced elongated ripples (500 Å), which finally span several micrometer (1000 Å). The low growth temperature of 425 °C influences growth as the number of accumulated defects is also increased with layer thickness. This shows up as holes and constricted bunches (Fig. 2, 3000 Å).

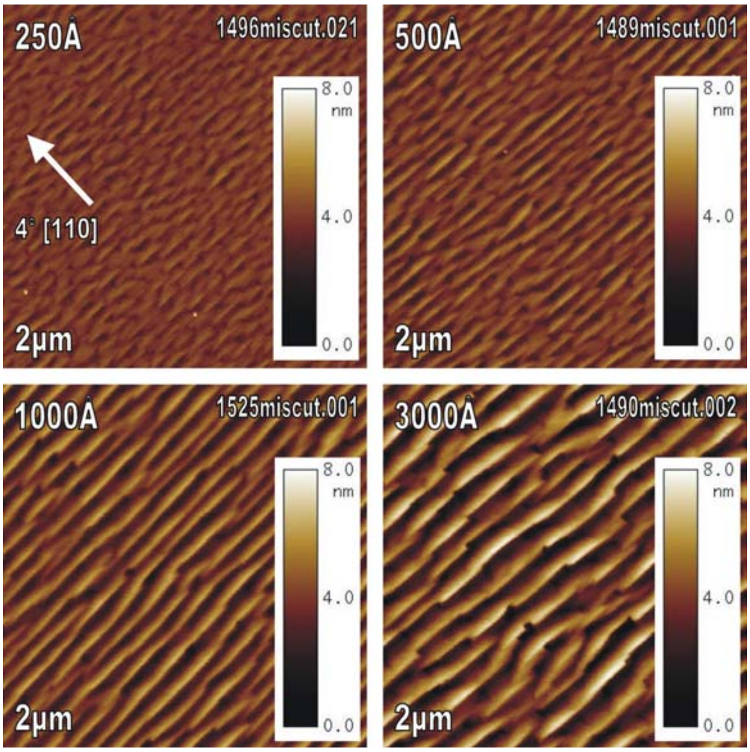

Fig. 2: AFM-images showing the layer thickness-dependence of step-bunching. The series of 250Å, 500Å, 1000Å and 3000Å thick Si-buffers grown on 4° [110] miscut samples (@ 0.2 Å/s Si) indicate that the ripple structure gets even more pronounced with increasing layer thickness. An increase in the period and the structure height of the step-bunches is clearly visible.

Further experiments were conducted with 1000 Å thick Si-buffers (@ 425°C, 0.2 Å/s Si), which show typical dimensions of 100 nm for the ripple period and 4 nm for the ripple height (miscut 4° [110]). Figure 3 shows the comparison and evaluation of AFM-data for a pure, 1000Å thick Si-buffer, and a Si-buffer covered with 50Å $Si_{0.55}Ge_{0.45}$ at 425 °C and 550 °C, respectively. In the case where the substrate-temperature was increased to 550 °C for the $Si_{0.55}Ge_{0.45}$ top-layer, the highly strained epilayer relieves stress forming {105}-faceted islands, which are known from the hut-clusters of relaxed SiGe-films. On our miscut-samples the islands are bound by two {105}- and the (001)-facet on top, while the underlying ripple pattern is widely conserved. Even at the low temperature of 425 °C the $Si_{0.55}Ge_{0.45}$ film does not replicate the underlying ripples of the Si-buffer in a conform manner. The stress in the top-layer leads to the formation of ridges at the ripple-flanks, perpendicular to the main structure. This marks the transition from conformal Si/SiGe epilayer growth [3] to strain-driven 3D-growth and is illustrated with 3D-AFM data in Fig. 3 (c). FFT evaluations reveal a period of approximately

100 nm for the step-bunches on the Si-buffer. The $Si_{0.55}Ge_{0.45}$ islands decorate the kinetic step-bunches, but have a somewhat smaller spacing of ~70 Å along the ripples (Fig. 3 (b)).

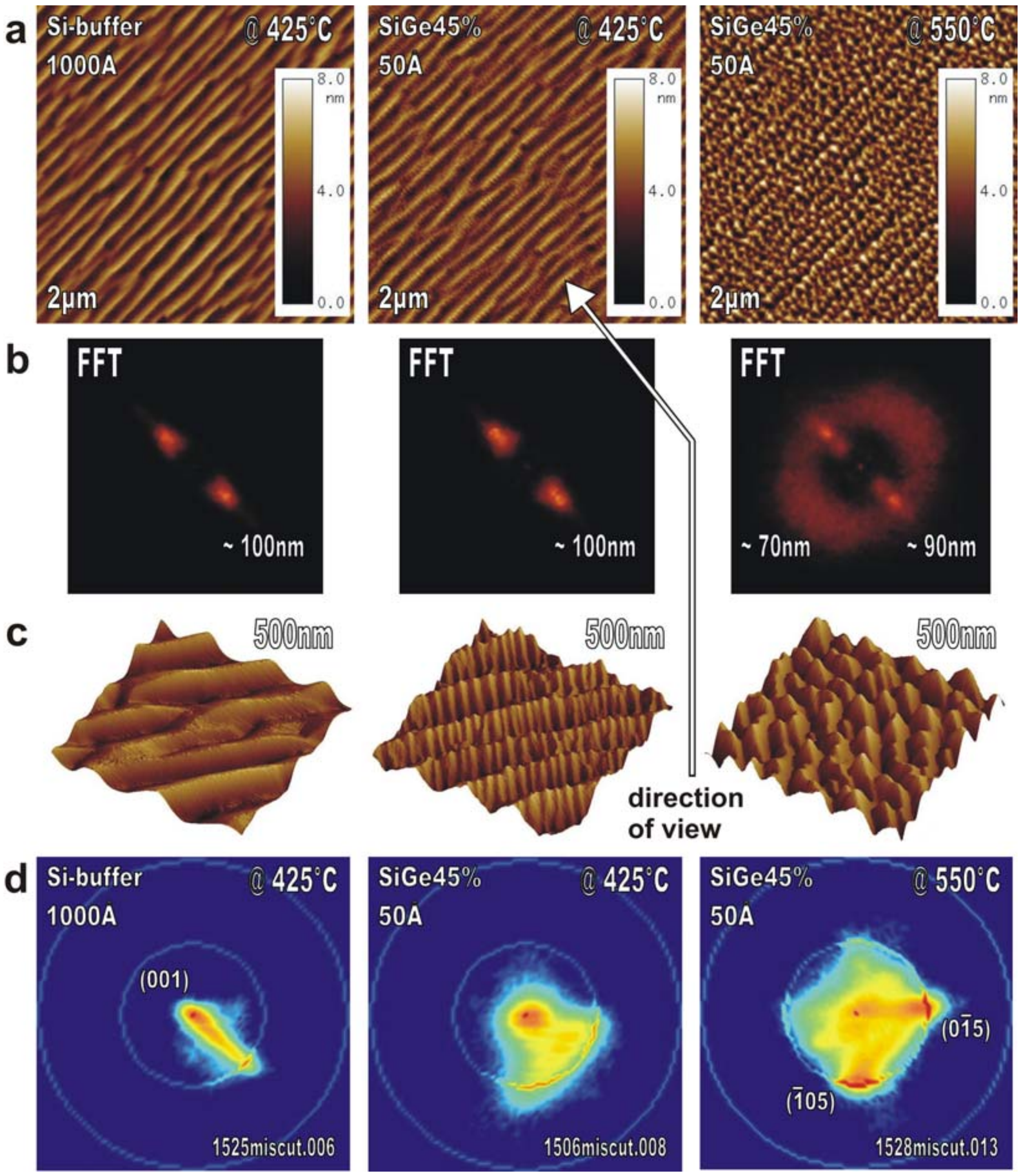

Fig. 3: AFM-data for the pure 1000 Å Si-buffer, the Si-buffer covered with 50 Å $Si_{0.55}Ge_{0.45}$ (all 4° [110] miscut) at 425 °C and 550 °C, respectively. Conventional 2D-AFM images (a) are completed with corresponding FFTs (b), 3D-AFM representations (c) and surface-orientation histograms (d) to illustrate the transition from pure step-bunching to {105}-faceted islands.

The individual facets of the islands are determined from a surface-orientation-histogram, which is derived from tilt-corrected AFM-data (Fig. 3 (d)).

In Fig. 4 a schematic drawing illustrates the faceted layer morphology next to distorted 3D-AFM data of the 50 Å $Si_{0.75}Ge_{0.25}$ 425 °C sample used for the surface normal vector analysis. The formerly straight steps with the flat terraces oriented in (001) direction and the flanks with angles of typical ~8° for Si-homoepitaxy are now confined by zigzag edges. As the slope of the ripples matches the angle of the intersection edge of two adjacent {105}-facets, these flanks form perfect nucleation sites for the highly strained SiGe-layers to relief strain. Therefore at medium temperatures ridges organize perpendicular to the step-bunching pattern (Fig. 4). For growth at 550 °C relaxed islands and asymmetric hut-clusters align in chains along the bunches and result in an ordered decoration of the step-bunching pattern.

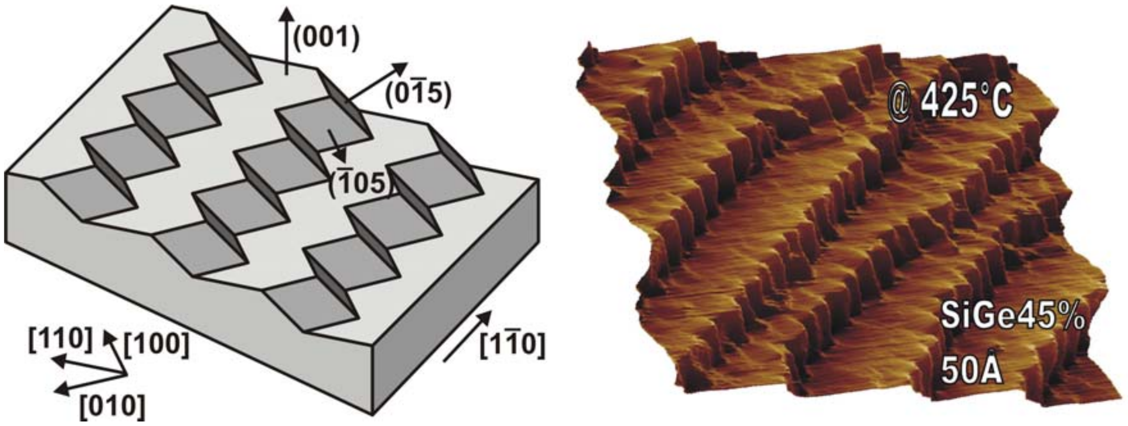

Fig. 4: Schematic drawing and 3D-AFM data for a 1000 Å Si-buffer covered with 50 Å $Si_{0.75}Ge_{0.25}$ at 425 °C. The distorted AFM-data representation (scan-size 500 nm) shows that the ripples with the (001)-oriented terraces exhibit a zigzag at the edges. The smooth flanks with typically ~8° with respect to [001] for homoepitaxy are energetically favourable nucleation sites for the strained SiGe-epilayer leading to a {105}-faceted ridge structure, which is perpendicular to the step-bunches.

By optimizing the growth parameters improvements in size-uniformity and ordering are expected [4].

Conclusion

Step-bunching is a purely kinetic growth instability which occurs during homoepitaxy on Si(001). For a miscut of 4° [110] the period of the ripple-pattern can be reduced to 90nm still exhibiting a height modulation of ~4 nm. Highly strained $Si_{0.55}Ge_{0.45}$ epilayers grown on top of such rippled Si-buffers reveal additional features by decomposing into faceted islands and decorating the underlying ripple-pattern in an organized manner.

Acknowledgements

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