

# MBE Growth Conditions for Si Island Formation on Ge(001) Substrates

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Here, we report on MBE growth conditions for Si island formation on Ge (001) substrates. After buffer layer growth Si deposition was varied from 6 to 20 ML in the temperature range from 400 to 550 °C. AFM and HRTEM images confirmed the Stranski-Krastanov growth of Si on Ge substrates.

## Introduction

In the Si/SiGe heterosystem self-organization schemes based on Stranski-Krastanov (SK) growth were mainly investigated for compressively strained Ge layers on Si substrates [1]. Because of the Type II band alignment this leads to hole confinement in the Ge islands, whereas tensely strained, Si-rich dots would be required for electron confinement. Little is known about SK growth of Si on Ge or SiGe, but there are strong indications that dot formation is kinetically hampered, if the epilayer is under tensile strain [2]. However, SK growth is driven by total energy minimization, which is independent of the sign of the lattice mismatch. And indeed, SK growth has been observed in heterosystems under tensile strain [3].

## Experimental Procedure

Here, we report on MBE growth conditions for Si island formation on Ge (001) substrates. The substrates were chemically pre-cleaned, followed *in-situ* by a 30 minutes outgassing step at 300 °C and by a thermal oxide desorption step. We optimized the growth conditions for the subsequent Ge buffer to get smooth surfaces with double atomic height steps only.

## Results and Discussion

On such buffers Si growth was initially investigated at 750 °C to stay close to thermal equilibrium. Under these conditions island formation was observed, which was, however, concomitant with strong alloying to average Ge compositions of up to 80% [4].

Lower growth temperatures drastically reduce alloying. We therefore investigated the formation of Si-rich islands in the temperature range from 400 to 550 °C with varying Si deposition from 6 to 20 monolayers. As an example, Fig. 1(a) – (d) shows a series of samples grown at 500 °C with Si coverages from 10 to 20 ML. In Fig. 1(e) the dot densities vs. Si deposition are plotted for four different growth temperatures. The steep increase in each curve allows for the extraction of the 2D-to-3D transition, which decreases from  $\approx 14$  ML at 550 °C to  $\approx 8$  ML at 450 °C, most likely due to more pronounced alloying at higher temperatures.

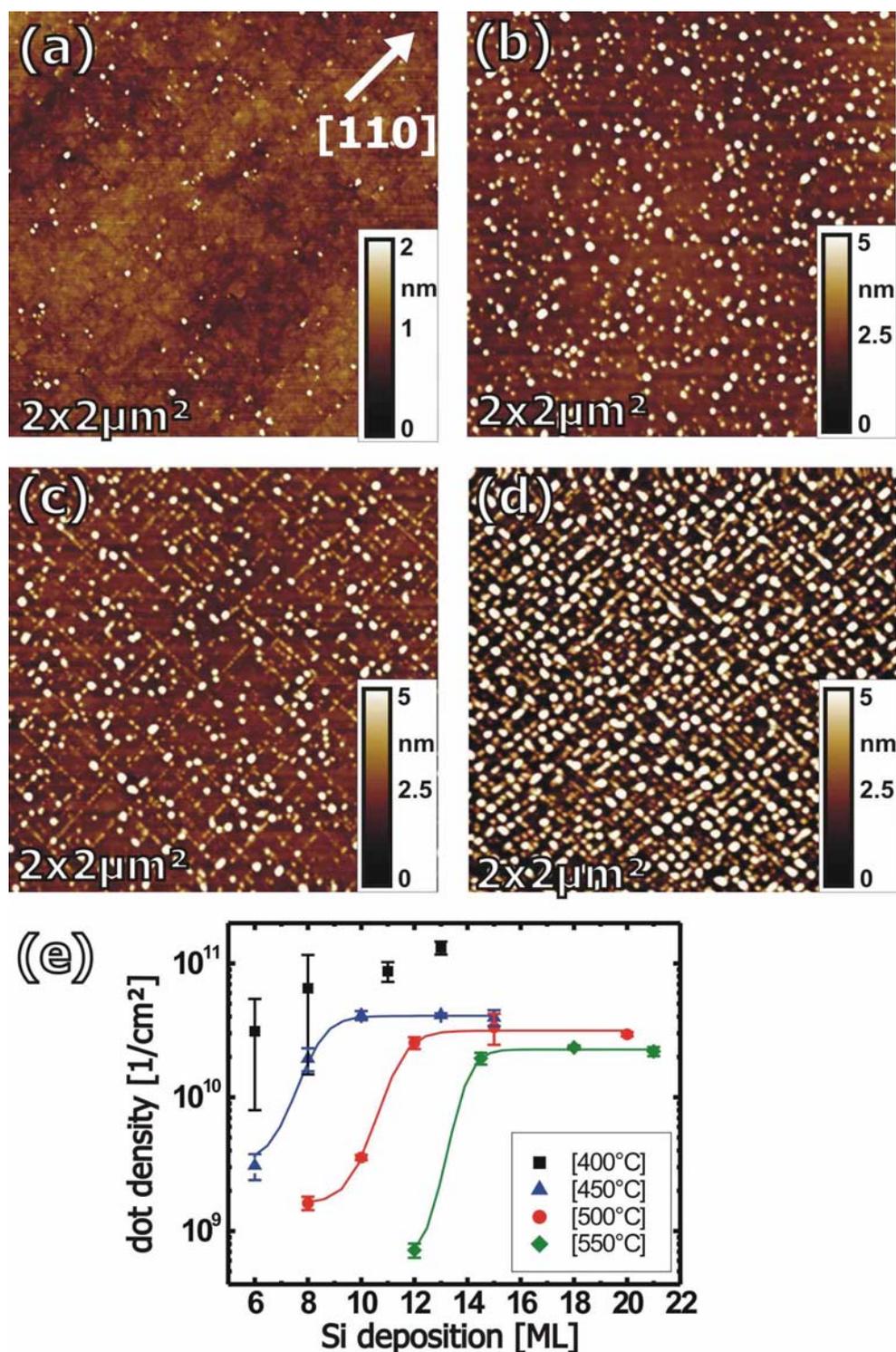


Fig. 1: AFM images of Si grown at 500°C with a varying ML deposition (a) 10 ML, (b) 12 ML, (c) 15 ML and (d) 20 ML; (e) dot density vs Si deposition as a function of growth temperature.

At 500 °C the wetting layer is about 10ML thick, a value which we also confirmed by high-resolution cross-sectional TEM (HRXTEM) images (Fig. 2). Evidently, the Si wetting layer on Ge is much thicker than the typical 3 ML found for Ge growth on Si, and, even worse, it reaches the equilibrium critical thickness for dislocation nucleation. It is therefore not too surprising that the HRXTEM images revealed dislocations already in

the wetting layer (Figs. 2(b) – (c)). Evidence for the presence of dislocations in the wetting layer can also be found in the AFM images in Figs. 1(c) – (d), which clearly show partial ordering of the Si islands along  $\langle 110 \rangle$  oriented lines. Most likely, these islands decorate misfit dislocation segments, as has also been observed for Ge on dislocated SiGe(001) pseudosubstrates.

Surface orientation maps show that the larger islands are truncated pyramids with  $\{113\}$  facets, whereas the small islands consist predominantly of facets orientations between  $\{117\}$  and  $\{1\ 1\ 10\}$ . These facets have inclination angles against the (001) substrate plane between  $8^\circ$  and  $11^\circ$ , and have also been found in earlier work on pit-patterned Si substrates after overgrowth with a Si buffer layer [5]. Compared to  $\{105\}$  faceted Ge pyramids on Si, the small Si islands have similar inclination angles of the sidewall facets, but are rotated by  $45^\circ$ .

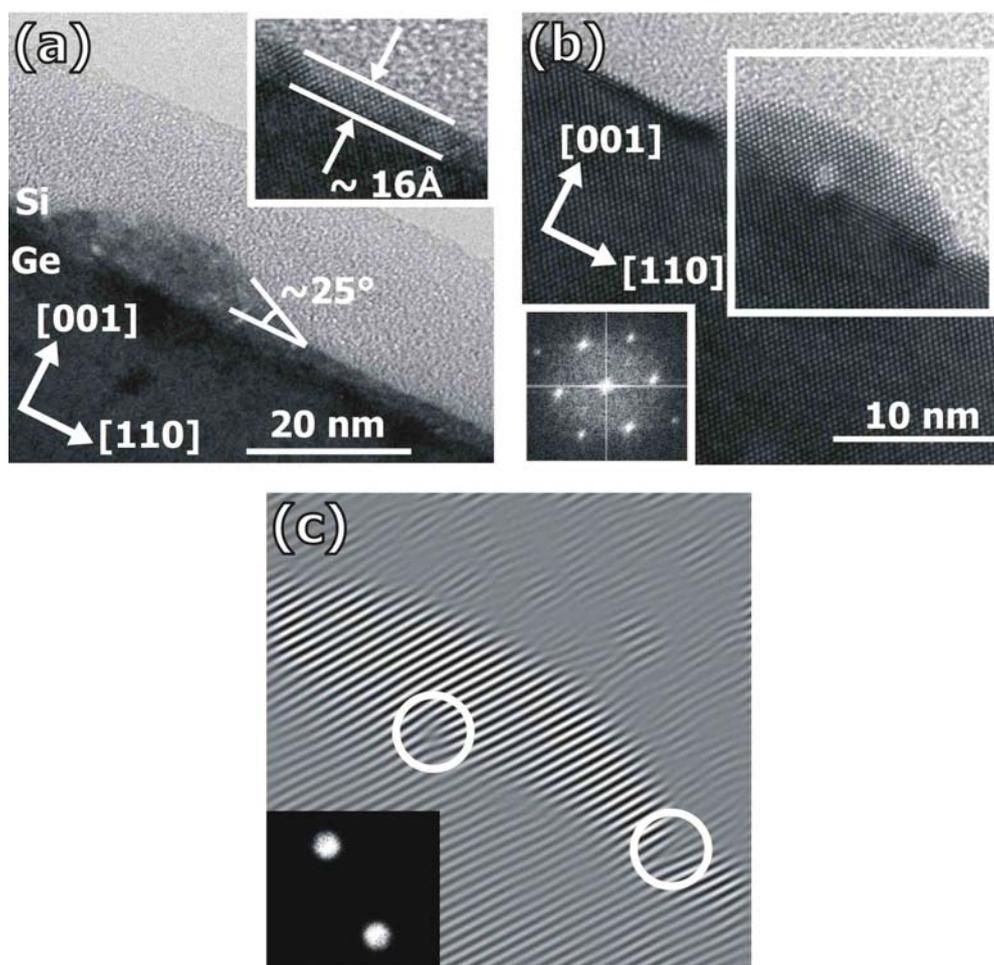


Fig. 2: Cross-sectional TEM images of 15 ML Si grown at  $500^\circ\text{C}$ ; (a) Si dot with  $\{113\}$  facets and wetting layer thickness of  $\sim 11$  ML ( $=16\text{\AA}$ ); (b) high resolution TEM image of a Si dot and wetting layer with dislocations; (c) filtered fast Fourier transformation (FFT) of the marked area in (b) showing two dislocations (circles).

## Summary

Our experiments clearly demonstrate that SK-growth of Si on Ge is possible. Further growth optimization is still required to suppress dislocation formation in the wetting layer.

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