Growth Instabilities in Si/SiGe Homo- and Heteroepitaxy

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We show that for a large set of growth parameters the reason for ripple formation in the Si/SiGe system is the kinetic step-bunching instability found in Si homoepitaxy. Single $Si_{1-x}Ge_x$ layers (with x around 0.5) do not show step-bunching. In superlattices, the instability has a similar behavior as the instability in homoepitaxy. Mainly the growth temperature influences the surface morphology; only little changes can be found when the germanium content in the superlattices is changed. In addition, the increase of ripple height and period with increasing amount of deposited silicon is similar to the one found in homoepitaxy. The more germanium is present in the superlattice the less pronounced the step-bunches appear. In kinetic Monte-Carlo simulations we show that only the interplay between diffusion anisotropy on the (2×1) reconstructed Si(001) surface and the attachment/detachment of adatoms on the step-edges is responsible for the growth instability in Si homoepitaxy.

Introduction

The Si(001) surface is the technologically most important surface for the semiconductor industry. The step-bunching growth instability on vicinal Si(001) is single $Si_{1-x}Ge_x$ layers and Si/SiGe superlattices was often believed to be strain-induced [1]. In fact, it has been found that a step-bunching instability resulting in an indistinguishable surface morphology appears already in Si homoepitaxy [2], where no strain is present.

Experiments

Single SiGe layers and Si/SiGe superlattices (SLs) have been grown by solid source molecular beam epitaxy (MBE) on RCA-cleaned substrates with a miscut of 0.66° in [110] direction to investigate the influence of germanium.

Single $Si_{1-x}Ge_x$ layers (with x around 0.5) do not show step bunching. They replicate the morphology of the underlying buffer layer, which can be chosen as flat or rippled by selecting proper growth conditions. These layers disintegrate into hut-clusters when allowed to reach thermodynamic equilibrium [3].

In superlattices the instability has a similar behavior as the instability in homoepitaxy. When miscut (0.66°) and growth rate (0.2 Å/s) are kept constant, mainly the growth temperature influences the surface morphology, only little changes can be found when the germanium content in the superlattices is changed (see Fig. 1). In addition, the increase of ripple height and period with increasing amount of deposited silicon is similar to the one found in homoepitaxy. Both follow a $y=a \cdot x^b$ type law, with critical exponents of 0.5 and 0.25 respectively. The more germanium is present in the superlattice the less pronounced the step-bunches appear. We attribute this slight decrease with in-

creasing germanium content to changes in surface kinetics, which are due to the segregation of germanium [4].

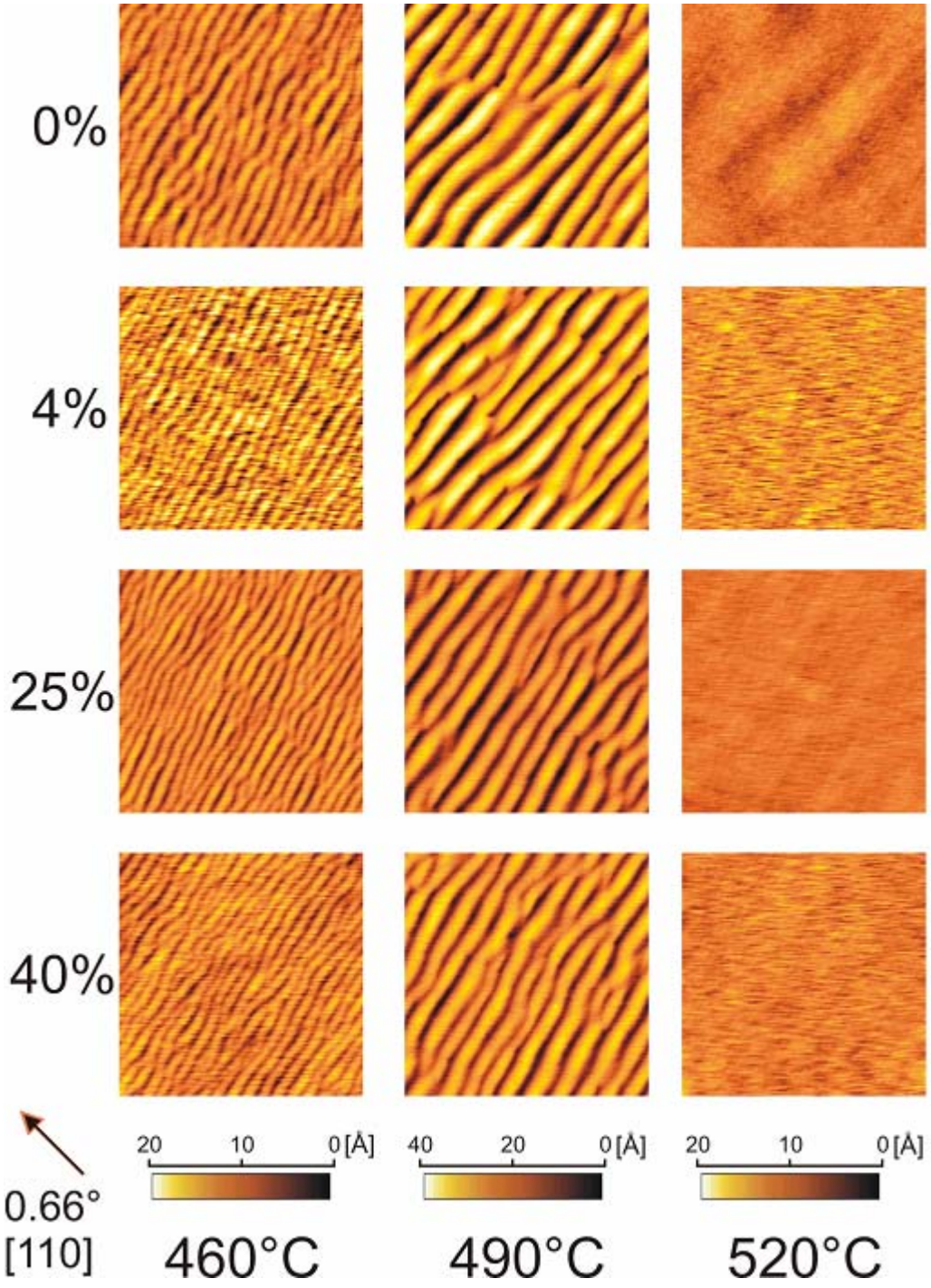

Fig. 1: AFM images of 10× [30Å Si / 300 Å $Si_{1-x}Ge_x$] superlattices grown at various growth temperatures (indicated on the bottom) and Ge-contents (indicated on the left). The miscut direction is given by the arrow on the lower left side. All images are 5×5 µm² in size.

Kinetic Monte-Carlo Simulations

In two-dimensional kinetic Monte-Carlo simulations, we show that growth kinetics is the mechanism, which is relevant for the step bunching. In Si homoepitaxy only the interplay between the diffusion anisotropy on the (2×1) reconstructed Si(001) surface and the attachment/detachment of adatoms on the different S_A and S_B step-edges is responsible for the growth instability in Si homoepitaxy. No step-edge barriers are necessary to explain the experimentally observed morphology [5]. Figure 2 shows images illustrating the time evolution of the sample surface during the simulation.

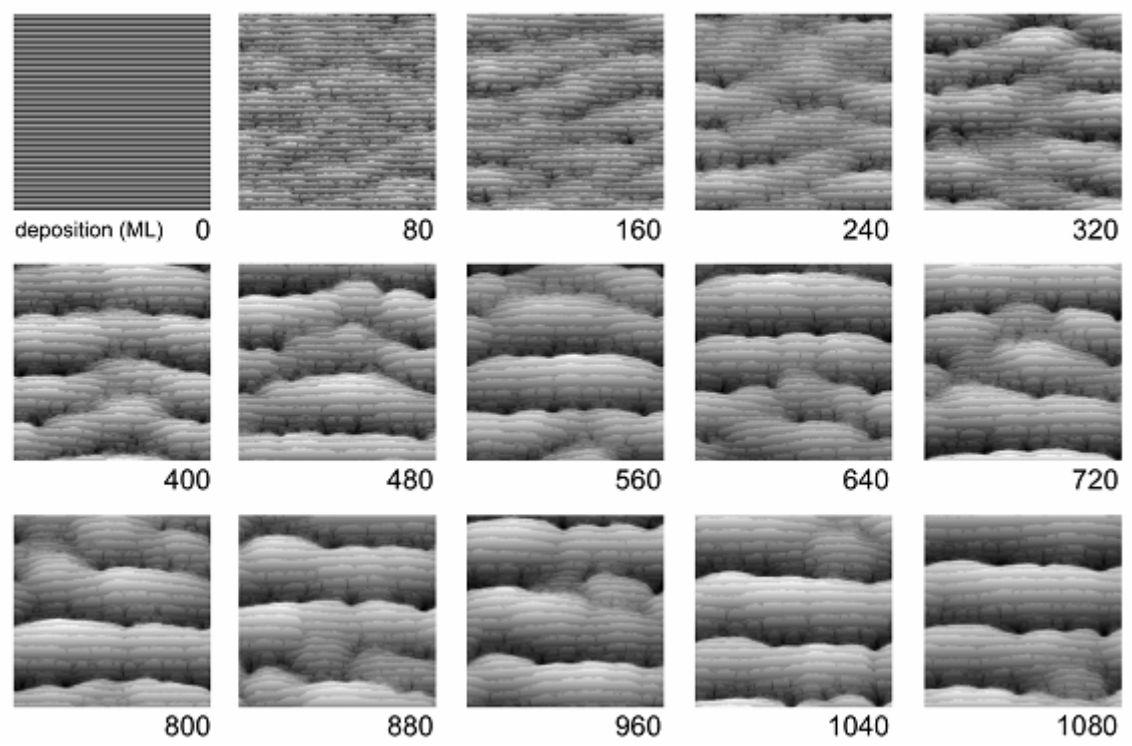

Fig. 2: Results of the two-dimensional kinetic Monte Carlo simulation showing the evolution of the surface. The number of deposited monolayers (MLs) is given for each image.

Conclusion

In conclusion, we show that for a large set of parameters strain-induced step bunching can be excluded with high probability and that the reason for ripple formation in the Si/SiGe system is only the kinetic step bunching instability found in Si homoepitaxy. We find that germanium slightly influences the step bunching in Si due to its segregation but not due to the strain introduced because of the lattice mismatch. Two-dimensional kinetic Monte Carlo simulations give close insight in the atomic mechanisms responsible for this phenomenon.

References

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