Investigations on the Wetting Layer and the Island Nucleation in the SiGe System on Planar Si(001) Substrates

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In this work investigations on the Ge profile along the growth direction in SiGe wetting layers (WL) grown on Si(001) substrates are presented. The high relative resolution (0.025 monolayer) of the sample series is used to monitor the dependence of the WL photoluminescence (PL) transition energies on the amount of deposited Ge. Fitting **k·p** band structure calculations to the almost linear confinement shift provides for the first time reliable quantitative Ge profiles in the WL. The importance of the Ge content and thus the strain in the WL on the island nucleation is shown.

Introduction

Due to its relative simplicity the SiGe system has acted as model system for understanding the hetero epitaxial growth of semiconductor nanostructures. Ge on Si (lattice mismatch of 4.2%) grows in the Stranski-Krastanow mode. Ge forms within the first monolayers of growth a thin film on the Si (001) surface, adapting the inplane Si lattice constant. As the Ge film grows thicker the strain energy in the Ge film is either reduced by plastic relaxation, leading to dislocation nucleation, or by elastic relaxation, relieving the strain by island formation. However, despite the huge research efforts fundamental properties like Ge concentrations in the WL that influence the strain in the Ge film are not quantitatively known. The atomic force microscopy (AFM) images in Fig. 1 highlight the influence of increased intermixing and thus strain at higher growth temperatures (T_G). For these samples, 6 ML of Ge were grown at different T_Gs, ranging from 500 °C to 750 °C. At elevated temperatures the SiGe intermixing becomes enhanced and therefore the strain in the layers is reduced. This leads to a drastic increase of the WL thickness and the island sizes which, as a consequence has a large influence on the optical and electrical properties of such islands.

Experimental

The samples used for determination of the WL profiles were grown by solid source molecular beam epitaxy (MBE) on 4 inch Si(001) wafers. A 450 Å thick Si buffer layer was grown at a rate of 0.6 Å/s while the substrate temperature was ramped up from 450 °C to 550 °C. Only for the subsequent deposition of Ge (growth rate: 0.05 Å/s, growth temperature: 700 °C), the substrate rotation was turned off to implement a shallow, monotonous gradient of deposited Ge across the wafer. The local variation of the deposited Ge was determined by x-ray measurements on reference samples, and varies linearly from -20% to +20% across the wafer with respect to the nominal value in the wafer center. Three series of samples were prepared for PL experiments, which received 500 Å thick capping layers deposited at a rate of 1Å/s and deposition temperatures (T_c) of 300, 500 and 700 °C, respectively. For the PL investigations the wafers were cut into

pieces along the Ge gradient, and up to 75 PL spectra per wafer were taken at 4.2 K. PL was excited with an argon ion laser operating at 514.5 nm with 1 W/cm^2.

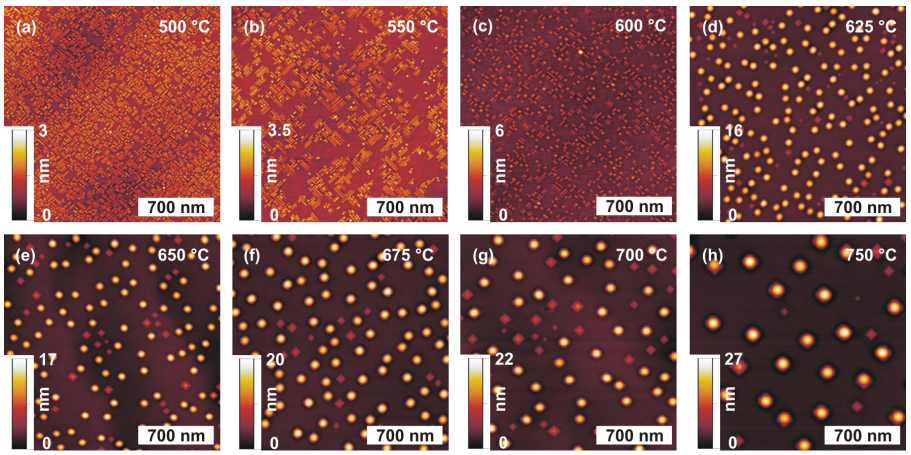

Fig. 1: AFM height images of Ge islands, deposited at different temperatures. (a) T_G = 500°C, (b) 550°C (c) 600°C (d) 625°C (e) 650°C (f) 675°C (g) 700°C and (h) 750°C. Despite the abrupt transition from (105) facetted hut clusters to the bi-modal pyramid-dome distribution between 600°C and 625°C, the increase of the island sizes with increasing T_G due to increased intermixing is obvious.

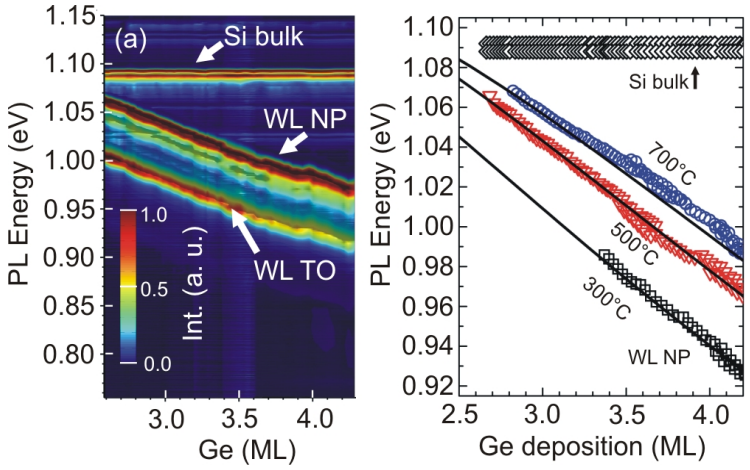

Fig. 2: (a) Dependence of the PL energies on the deposited amount of ML of a sample series grown at 700 °C and capped at 500 °C. The corresponding intensities of the WL and substrate peaks are color coded (b) Black open squares, red open triangles and blue open circles correspond to different T_cs of 300 °C, 500°C and 700°C. The Ge WL was deposited at 700°C for all samples. The black solid indicate the fitted confinement shift for the WL Ge profiles shown in Fig. 4.

Results

In Fig. 2 (a), normalized PL spectra are shown for the samples with at T_c = 500 °C. The WL emits characteristic quantum well (QW) PL bands consisting of a spectrally narrow no-phonon (WL NP) line and its split-off Si-Si TO phonon replica, (WL TO^{Si-Si}). With Ge coverage increasing from 2.6 ML to 4.3 ML, the WL bands shift to lower energies, be-

cause the confinement energy decreases with increasing WL thickness. Due to the shallow gradient of the Ge coverage across the wafers, the shift could be monitored with the extremely high resolution of 0.025 ML. Figure 2 (b) summarizes from a set of 10 wafers the dependence of the WL_{NP} energies on Ge coverage for the three investigated T_c's. A virtually linear decrease of the WL PL peak position with Ge coverage is observed for each T_c. Figure 2 (b) shows that the WL_{NP} peak positions shift to higher energies with increasing T_c. Since the WL was deposited under identical conditions on all samples, the observed shift of the WL_{NP} line indicates increased intermixing of the WL with increasing T_c. To determine the WL composition profile, and its dependence on T_c, we compared the PL results with band structure calculations. Since the band alignment of SiGe on Si(001) is of type II, only holes are confined to the WL. We calculated the heavy hole (HH) ground states in the WL on the base of a one band **k·p** envelope function model including the strain in the WL. Thus, the only two parameters, the HH effective confinement mass m_{HH}, and the valence band (VB) offset ΔV_{HH} enter [1]. The resulting values for m_{HH} decrease with only a small bowing from 0.276 m_o for pure Si to 0.223 m_o for $Si_{0.5}Ge_{0.5}$, and to 0.18 m_o for pure Ge. ΔV_{HH} increases linearly from 0 for pure Si to 720 meV for pure Ge. The WL_{NP} PL transition energy is calculated from the HH ground state energy by subtracting the energy difference between the HH ground state in the WL and the HH VB edge of bulk Si from the fundamental Si band gap. The seemingly linear slopes of the transition energies are due to the extremely narrow WL, which leads to ground state energies approaching the rim of the valence band QW.

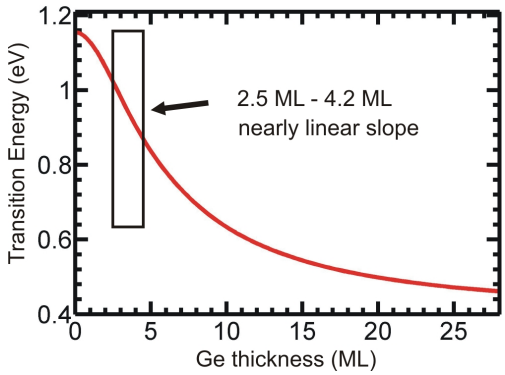

Fig. 3: Dependence of the transition energy on the thickness of a square quantum well with 100% Ge.

As shown in Fig. 3, at around 5 ML WL thickness, the thickness dependence of the WL PL energy shows vanishing curvature between the pinning to the QW rim and a $1/d_{WL}^2$ variation for QWs with large thickness d_{WL}. For a more realistic Ge profile, segregation and diffusion at both WL interfaces were taken into account. Four fitting parameters were used to model the shape of the hole-confining potential (i) The maximum Ge content x_{max} in the well, (ii) Si segregation at the lower interface, (iii) Ge segregation at the upper interface and (iv) Ge bulk diffusion, which is virtually negligible at the used T_cs. The observed blue shift of the WL PL energies with increasing T_c can only result from intermixing of the Ge WL with the Si cap due to segregation. For the high Ge concentrations in the WL, surface segregation results in an exponential composition profile at each interface with decay lengths λ_1 and λ_2 for the bottom and top WL interfaces, respectively. λ_1 was kept constant, because the lower interface was grown at 700 °C for all samples. λ_2 was varied with the cap deposition temperature T_c. In addition, a small amount of Ge bulk diffusion was allowed to smear out the sharp features in the concentration profiles. Good fits of the slopes for all T_c's (Fig. 2 (b)) could only be achieved for non-vanishing bulk diffusion length, and decay length λ_1. However, variations of L and

λ_1 within a realistic range of 0.5 Å < L < 2.5 Å and 0.1 < λ_1 < 0.3 have only negligible influence on the calculated binding energies of the WL quantum well. In the following, we used L = 1.3 Å and λ_1 = 0.25 Å. The two remaining fitting parameters are then x_{max}, and the segregation constant for the top interface, λ_2. The resulting Ge profile was used to calculate the spatial variations of strain and the HH valence band edges, the respective ground state energy in these potentials and the PL transition energies. The results shown by the solid lines in Fig. 2 (b) were obtained with x_{max} = 0.86 ± 0.01 and λ_2 = 1; 3.7; 4.8 Å for T_c = 300; 500; 700 °C. We want to point out, that by adjusting λ_2 only, both the change of the slopes and the relative positions of the three traces in Fig. 2 (b) are in excellent agreement with the experiment.

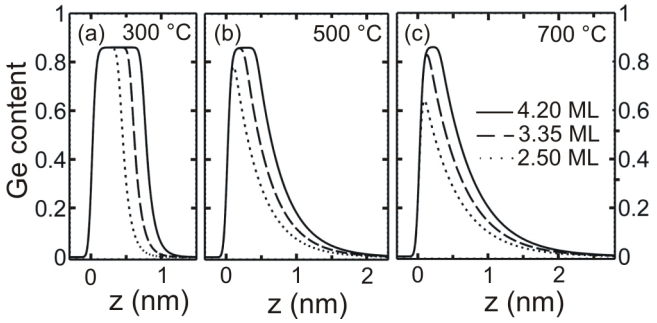

Fig. 4: Calculated Ge profile across the WL for T_c's of (a) 300 °C, (b) 500 °C and (c) 700 °C for the different Ge coverages indicated in the plot. The parameters for the calculated Ge profiles are: x_{max}= 0.86, L=1.3 Å, λ_1 = 0.25 Å, and λ_2 = 1; 3.7; 4.8 Å in (a), (b) and (c), respectively.

In Fig. 4, the results for the Ge profiles are shown for the three investigated T_c values. At T_c = 300 °C, an almost box-like Ge profile is obtained, indicating negligible Ge segregation. Increasing T_c to 500 °C and 700 °C results in enhanced Ge segregation, as indicated in Figs. 4 (b) and (c) by the decaying Ge profiles. The large value obtained for x_{max} evidently depends to some extent on the alignment of the Si and SiGe valence bands in the calculations. We checked the dependence of the result for x_{max} on the valence band alignment ΔV_{HH} and obtained a sensitivity of $\Delta x_{max}/\Delta(\Delta V_{HH}) = 2.4 \times 10^{-3}$ (meV^{-1}).

Conclusion

We have performed a detailed investigation of the dependence of the PL emission of a Ge WL on the amount of deposited Ge. By freezing the substrate rotation during Ge deposition, we were able to study systematically the shift of the WL emission as a function of Ge coverage with 0.025 ML resolution. These data allowed for an unambiguous fit of the observed slopes dE_{WL}^{NP} / dd_{WL} to results of band structure calculations. From these fits we determined quantitative Ge profiles along the growth direction and their dependence on T_c. At T_c = 300 °C an almost box-like Ge profile of the WL is obtained with a maximum Ge concentration of 86%. For Ge coverages > 4.2 ML this large maximum Ge concentration is preserved also in WLs capped at 500 °C and 700 °C.

References

[1] M. Brehm et al., Applied Physics Letters, **93**, (2008)