Si passivation of epitaxial SiGe: kinetics and impact on morphology

Birgit Seiss^{1,2} and Didier Dutartre¹ ¹STMicroelectronics, 850 Rue Jean Monnet, 38926 Crolles Cedex, France; birgit.seiss@st.com ²Institut des Nanotechnologies de Lyon, 7 Av. Jean Capelle, 69621 Villeurbanne Cedex, France

 $Si_{1-x}Ge_x$ (SiGe) epitaxy is used in CMOS technologies, in conventional and advanced architectures, to realize for example high mobility channels, embedded or raised sources/drains. With each node the feature size decreases, leading to an increased sensitivity of SiGe to thermal budgets. Indeed, we recently showed that the SiGe morphology is extremely sensitive to temperature [1]. Passivating the surface with Si could be an option to make the SiGe more temperature-resistant. Si passivation may also be used to eliminate the observed difference of the oxidation rate between Si and SiGe surfaces [2]. In this study, the passivation layer characteristics and its effect in terms of temperature resistance are reported.

In first experiments, 15 nm of epitaxial $Si_{0.72}Ge_{0.28}$ were grown on Si (001) substrates by rapid thermal chemical vapor deposition at 600°C using a mixture of SiH₄, GeH₄, HCl and H₂ gases. Directly after epitaxy, the SiGe was passivated in-situ by a SiH₄ + HCl + H₂ treatment for 20, 55, 110 and 220 s. X-ray photoelectron spectroscopy (XPS) measurements were subsequently performed in order to characterize the Si passivation layer.

Fig. 1 shows the Ge2p_{3/2} and Ge3d peaks of all passivated wafers as well as the peaks of one SiGe reference wafer without Si passivation. The peak intensity is lower for the passivated wafers compared to the reference wafer and it decreases with increasing passivation time. Based on these peak intensities the passivation thickness th can be calculated by the following equation: th=-sin(α) $\lambda \ln(I/I_0)$; where I and I₀ are the intensities of the passivated wafer and reference wafer, respectively, α is the take-off angle and λ the mean free path of Ge2p_{3/2} or Ge3d photoelectrons in Si. For both, the $Ge2p_{3/2}$ and Ge3d peaks, the same thicknesses are obtained at a given passivation time. In Fig. 2 the passivation thickness is plotted as a function of time t, revealing a non-linear dependence. Therefore, as a first approach, the growth rate (GR) is calculated as $\Delta th/\Delta t$ between two adjacent points. A significant decrease of the GR during the first ~40 s can be observed in the plot GR vs. time in Fig. 2. For longer passivation times, the GR continues to decrease but more moderately. An explanation for this non-constant GR is the rising coverage of the SiGe layer by Si atoms. Hydrogen desorption, which is limiting the growth at low temperatures, is catalyzed by Ge atoms [3]. Consequently, the GR decreases when the Ge atoms are covered by Si atoms due to the loss of this catalytic effect.

In the next experiments, two patterned wafers with a passivation of 20 and 110 s were annealed at 750°C under 10 Torr of H₂ for 60 s, in order to study the influence of passivation on the morphology change during annealing. Atomic force microscopy (AFM) images at the edge of a pattern are displayed in Fig. 3. After annealing, the morphology of 20 s passivated SiGe is quite similar to non-passivated SiGe. This means that the formation of ridges due to the Stranski-Krastanov (SK)-like strain relaxation in the pattern interior and the recently reported edge effect at the pattern boundaries [4] can be observed. Passivation of 110s inhibits the SK-like strain relaxation, whereas it plays only a minor role on the edge effect. Fig. 4 compares the height profiles perpendicular to the edge for both passivation times. The peak-to-valley value of the edge changes from 16 to 9 nm, upon increasing the passivation time from 20 to 110 s. The different impact of the passivation on the SiGe morphology regarding the SK-like strain relaxation and edge effect will be addressed in the final paper.

References:

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Figure 1: $Ge2p_{3/2}$ (left) and Ge3d (right) XPS spectra for a passivation time of 0, 20, 55, 110 and 220 s.



Figure 2: Si passivation thickness (left axis) and growth rate (right axis) as a function of passivation time.



Figure 3: $2x2 \mu m$ AFM height images at the edge of a $300x300 \mu m$ pattern. The passivation times are 20 s (left) and 110 s (right).



Figure 4: Height profiles taken perpendicular to the pattern edges of Fig. 3.