Relaxed SiGe-on-insulator fabricated by dry oxidation of sandwiched Si/SiGe/Si structure

Zengfeng Di a,b, Miao Zhang a, Weili Liu a, Ming Zhu a,b, Chenglu Lin a, Paul K. Chu b,*

a The Research Center of Semiconductor Functional Film Engineering Technology & State Key Laboratory of Functional Materials for Informatics, Shanghai Institute of Microsystem and Information Technology (SIMIT), Chinese Academy of Sciences (CAS), Shanghai 200050, People’s Republic of China
b Department of Physics and Material Science, City University of Hong Kong, Tat Chee Avenue, Kowloon, Hong Kong, China

Abstract
An improved technique is demonstrated to fabricate silicon–germanium on insulator (SGOI) starting with a sandwiched structure of Si/SiGe/Si. After oxidation of the sandwiched structure and successive annealing, a relaxed SiGe-on-insulator (SGOI) structure is produced. Our results indicate that the added Si cap layer is advantageous in suppressing Ge loss at the initial stage of SiGe oxidation and the subsequent annealing process homogenizes the Ge fraction. Raman measurements reveal that the strain in the SiGe layer is fully relaxed at high oxidation temperature (∼1150 °C) without generating any threading dislocations and crosshatch patterns, which generally exist in the relaxed SiGe layer on bulk Si substrate.

© 2005 Elsevier B.V. All rights reserved.

Keywords: SiGe-on-insulator; Oxidation; Diffusion

1. Introduction
Strained Si with in-plane tensile strain on (001) relaxed SiGe is a promising substrate for high-performance metal-oxide-semiconductor field-effect transistors (MOSFETs) because both the electron and the hole mobilities are enhanced [1,2]. Similarly, incorporation of silicon-on-insulator (SOI) into MOSFETs gives rise to advantages including reduced parasitic capacitance, increased circuit density due to tighter isolation, and reduced short-channel effect as well as latch-up [3]. Therefore, the combination of strained Si layers on relaxed SiGe-on-insulator has attracted much interest due to the combined advantages of these two complementary technologies [4,5].

To take advantage of strained-CMOS, a technique to fabricate high-quality relaxed SGOI must be established. Huang et al. utilized an ultra-thin SOI as a “compliant substrate” to partially relax an initially strained SiGe film [6,7]. An et al. carried out separation by implantation of oxygen (SIMOX) on a strained-relaxed SiGe virtual substrate [8,9]. Huang et al. [10] used the Smart-Cut™ technique to transfer a layer of SiGe onto the oxide. However, most SGOI layers fabricated by these methods do not meet the application requirements as they are too thick and/or have too low a Ge fraction. Recently, Tezuka et al. proposed a novel SGOI fabrication technology based on Ge condensation by oxidation of the SiGe layer on a SOI layer [11]. There is, however, one intrinsic problem about Ge loss in this method. Firstly, although the free energy of formation of SiO₂ is much lower than that of GeO₂ [12] and SiO₂ is preferentially produced rather than GeO₂, according to a diffusion model [13] the silicon flux is considerably smaller than the oxygen flux at the initial stage of SiGe oxidation and so the formation of mixed (Si, Ge)O₂ or SiO₂–GeO₂ [14–16] is difficult to avoid. Secondly, the formation of volatile GeO is relatively easy and it diffuses out before a complete layer of SiO₂ is formed to prevent further loss [17,18] at the early stage of SiGe oxidation.

In this work, we modify the conventional condensation technique to fabricate SGOI throughout the oxidation of a sandwiched structure Si/SiGe/Si. The added Si cap is advantageous to solving the problem mentioned above.

2. Experimental details

The modified SGOI fabrication procedures are schematically illustrated in Fig. 1. The starting SIMOX SOI wafers had a 30 nm thick top Si layer. A 100 nm SiGe epilayer with a uniform...
Ge composition of 18% was first pseudomorphically grown on the SOI substrate using SiH₄ and GeH₄ precursors. In order to avoid the formation of GeO, mixed (Si, Ge)O₂, or SiO₂–GeO₂ during the subsequent oxidation processes, GeH₄ was shut off and an added Si cap about 20 nm thick was produced on top of the SiGe layer as a modification to the conventional Ge condensation technique. The samples were oxidized for 1 h at 1150 °C in 100% oxygen ambient. Initially, the Si cap was oxidized to form a complete layer of SiO₂. When the oxidation front reached the buried SiGe layer, the SiO₂ layer reduced the oxygen flux and suppressed possible GeO volatilization. Meanwhile, an added Si cap ensured that the silicon flux was larger than the oxygen flux. The free energy of formation of SiO₂ is much lower than that of GeO₂ and therefore, Si atoms were preferentially oxidized rather than Ge atoms, and Ge atoms were rejected from the SiGe oxide layer. Consequently, the interface between the SiGe and SOI layers disappeared, while the average Ge fraction in the merged layer increased because Ge diffusion out of the layer was blocked by the top thermal oxide and BOX layer. Different from the conventional Ge condensation technique, the oxidized sample was annealed in N₂ for 3 h at 900 °C to homogenize the Ge fraction in the SiGe layer. After removing the surface oxide layer by diluted HF, a relaxed SGOI virtual substrate with a uniform Ge profile was fabricated without introducing dislocations.

3. Results and discussion

In order to determine the Ge loss via the formation of GeO₂, we conducted high resolution XPS measurement and then acquired the Si₂p and Ge₂p₃/₂ spectra at the interfacial region between the top oxide and SiGe films, as shown in Fig. 2. After the top SiO₂ has been sputtered by Ar⁺ ions, strong signatures of pure Si and SiO₂ bonding, namely Si₂p peaks at 99.3 and 103.3 eV [19], respectively, are observed in Fig. 2(a). The coexistence of pure Si and SiO₂ indicates that the XPS signals are from the region of the top oxide/SiGe interface. No Ge–O bonding peak at 1220.4 eV is detected. Only one XPS peak related to the Ge⁺ state of the SiGe layer appears at 1217.2 eV in Fig. 2(b), indicating no GeO₂ formation during oxidation. The main reason for germanium not participating in the reaction with O₂ is the more negative free energy of formation of SiO₂ compared to that of GeO₂ [12]. On the other hand, the added Si cap is advantageous to the suppression of the formation of GeO₂. From the perspective of a diffusion model concerning the oxidation behavior of SiGe alloys [13], a shift from SiO₂ to mixed (Si, Ge)O₂ or SiO₂–GeO₂ formation depends on the competition between the oxidant and silicon fluxes to the advancing oxide interface. At the early stage of SiGe oxidation, an added Si cap supplies an adequate silicon flux to react with the arriving oxygen flux,
Fig. 3. High-resolution TEM images of the fabricated SGOI structure. The Ge profiles across the layer measured by EDS are also shown.

Fig. 3 displays the cross-sectional TEM image of the fabricated SGOI structure and the Ge profile across the layers obtained by energy-dispersive X-ray spectrometry (EDS) using a CM200FEG system. It is found that the 30 nm thick top Si of the original SOI substrate has morphed into a SiGe layer which is about 95 nm thick. The clear lattice images shown in the TEM picture indicate that the rejected Ge atoms from the SiGe-oxide layer are located at the lattice points giving rise to no threading dislocation. The Ge fraction is about $x = 0.18 \pm 0.01$ with good uniformity. The fact that the final $x$ value almost coincides with $x_0(T_f/T_i) = 0.19$ [20] indicates that the total amount of Ge in the initial SiGe layer is conserved through the oxidation process. Here $x_0$ is the fraction of initial SiGe layer, $T_i$ the thickness of initial SiGe layer and $T_f$ is the thickness of final SiGe layer. Our results show that Ge loss by the formation of GeO$_2$ or GeO is effectively suppressed.

Fig. 4 compares the high resolution XRD results acquired from the following samples: (a) no oxidation but annealed at 1000 °C for 20 min and (b) 1 h oxidation at 1150 °C. The as-deposited sample was annealed at 1000 °C to relax the strain in the SiGe layer. In Fig. 4(a), the narrow diffraction peak located at 34.18° indicates that the as-deposited SiGe layer with 18% Ge is relaxed and has good crystal quality. Due to a small gradient of the Ge profile in the 1 h oxidized sample, the SiGe peak becomes a little broader compared to the as-deposited one with annealing, as shown in Fig. 4(b). Because the fabricated SGOI substrate has no obvious variation in the Ge concentration as confirmed by EDS measurement, the SiGe peak location does not change.

The surface morphology observed by atomic force microscopy (AFM) on the SGOI surface after removal of the surface oxide layers by HF etching is depicted in Fig. 5. The absence of crosshatch patterns, which is commonly observed on the surface of a relaxed or partially relaxed SiGe layer on a bulk Si substrate because of misfit dislocations [21], indicates that the
strain in the SiGe layer is relaxed without generating dislocations in the oxidation process. The root-mean-square roughness of the 1 h oxidized sample surface is estimated to be 2.8 nm, much smaller than a typical value of $\sim 10$ nm for a relaxed SiGe surface on bulk Si substrate [22].

In order to evaluate the degree of lattice relaxation, Raman measurements were carried out. Fig. 6 shows typical spectra in the range of 200–600 cm$^{-1}$ acquired from the fabricated SGOI substrate. The shifts of the Si–Si phonon peak can be clearly observed. The peak at $\sim 506$ cm$^{-1}$ is associated with the Si–Si vibration mode in the SiGe film. The Si–Si phonon peak from the Si substrate of the original SOI emerges at $\sim 519$ cm$^{-1}$. The Si–Ge vibration peak appears at $\sim 404$ cm$^{-1}$, and the weaker peak at $\sim 287$ cm$^{-1}$ is attributed to Ge–Ge motion in the SiGe layer. All modes are sensitive functions of the SiGe layer composition and the stress. For $x \leq 0.2$, the relative shifts of the Si–Si phonon mode of the SiGe layer from the Si substrate peak at room temperature can be described as a function of Ge fraction, $x$, by [23]:

$$
\begin{align*}
\Delta p.a. &= 69.0x \text{ (cm}^{-1}) \, \text{(full-relaxed)} \\
\Delta s.l. &= 36.0x \text{ (cm}^{-1}) \, \text{(full-strained)}
\end{align*}
$$

(1)

Here, $\Delta p.a.$ is the phonon shift of the fully-relaxed pseudo-alloy and $\Delta s.l.$ is that of the fully-strained superlattice SiGe alloy. The strain ratio, $S$, can be determined from the experimental shift of Si–Si Raman peak of SiGe film relative to the Si substrate value ($\Delta_{\text{exp}}$):

$$
S = \frac{\Delta_{p.a.} - \Delta_{\text{exp}}}{\Delta_{p.a.} - \Delta_{s.l.}}
$$

(2)

From Fig. 6, we derive that the strain ratio $S$ is 5.0%, which indicates that the strain in SiGe film is almost fully relaxed during high temperature oxidation. Strain relaxation in the SiGe layer can be explained by a simple model involving a compliant substrate [24]. During the oxidation process at 1150 °C [67.3% of the melting point of SiO$_2$ which is 1710 °C], the BOX layer becomes compliant and viscous. The shear stress which originates in the compressive strain in the SGOI layer can overcome the sticking force between the SiGe layer and BOX layer, thereby enabling the lateral expansion of the SiGe layer via an ultra-low viscosity slippage plane at the SiGe/BOX interface [25]. The compressive strain in the SiGe layer is thus relieved completely without the introduction of threading dislocations and crosshatch patterns.

4. Conclusion

Dislocation-free and strain-relaxed SGOI structure without crosshatch patterns on the surface was obtained by oxidation of a sandwiched Si/SiGe/Si structure at high temperature. Different from the conventional condensation technique, the added Si cap layer helps to suppress Ge loss via the formation of GeO$_2$ or GeO. The strain in the SiGe layer is almost fully relaxed during high temperature oxidation. This modified technique has high potential to produce ideal SGOI for strained CMOS applications in future technology nodes.

Acknowledgements

This work was jointly supported by the City University of Hong Kong Strategic Research Grant (SRG) 7001820, Shanghai Rising-star program no. 04QMX1463, the Special Funds for Major State Basic Research Projects G2000036506, and the National Natural Science Foundation of China under Grant Number (90101012 and 60476006).

References