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Self-limiting oxidation of SiGe alloy on silicon-on-insulator wafers

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Self-limiting oxidation of SiGe alloy on silicon-on-insulator wafers was investigated. For oxidation at 1000 °C, oxidation stops completely after a few hours for the $Si_{1-x}Ge_x$ (x=0.068–0.16) layers. For higher initial Ge concentrations of the SiGe layer, the oxidation saturated in a shorter oxidation time, whereas saturation was not observed for the oxidation at 900 and 1100 °C. The authors propose a model for self-limiting oxidation, in which the oxidation saturation is governed by an interfacial Ge-rich layer that depends on the oxidation temperature and the initial Ge concentration. © *2006 American Institute of Physics*. [DOI: 10.1063/1.2353812]

Recently, oxidation of SiGe alloy has been employed in the fabrication of SiGe-on-insulator (SGOI) substrates.[1,2] A strained Si layer is epitaxially grown on a relaxed SiGe surface, and it is used as the channel for metal insulator semiconductor field effect transistors (MISFETs). Devices which have a strained Si channel are expected to be used as high-speed MISFETs, because carrier mobility in strained Si is higher than that in relaxed Si.[3,4]

In the oxidation process of SiGe alloy Ge atoms are ejected from the interface between the surface oxide and the SiGe layers into the SiGe substrate. During the oxidation of the SiGe layer on the silicon-on-insulator (SOI) substrate, Ge atoms accumulate at the SiO_2/SiGe interface and diffuse towards the bottom of the SiGe layer. The concentration of Ge in the layers between the top oxide layer and the buried oxide (BOX) layer increases on further oxidation. It is considered that this Ge-condensation method produces a relaxed and thin SiGe layer with a high Ge fraction and low dislocation density, because the Ge concentration in the initial SiGe layer is sufficiently low to suppress dislocation and the slippage at the BOX layer interface occurs during condensation.[1]

It is, therefore, important to understand the oxidation mechanism of SiGe alloy. A considerable number of studies have reported the enhancement of the oxidation rate of SiGe alloy compared with that for pure Si.[5] However, there have been very few studies done on the reduction in the oxidation rate, as observed by Eugéne *et al.*[6] and Tezuka *et al.*[1] In this present study we investigated this reduction in the oxidation rate and observed self-limiting oxidation of SiGe alloy on a SOI wafer. We present the experimental evidence for this self-limiting oxidation of SiGe alloy and discuss the mechanism for this phenomenon.

Bonded SOI wafers with a 60 nm top Si layer and a 140 nm BOX layer were used as the starting substrate. The $Si_{1-x}Ge_x$ layers (x=0–0.16) with an average thickness of 188 nm were epitaxially grown on the SOI substrate in a molecular-beam-epitaxy chamber with an electron gun for evaporating Si and a Knudsen cell for evaporating Ge. The substrates were maintained at 480 °C during growth. Condensation of Ge was carried out by repeating oxidation at 900–1100 °C for 1 h in a 100% dry-O_2 atmosphere. The thickness of the oxide layer and the Ge concentration of the SiGe layer were measured by spectroscopic ellipsometry after each oxidation cycle. In order to obtain the depth profile of the Ge concentration, x-ray photoelectron spectroscopy (XPS) was employed using Ar^+ sputter etching after removing the surface oxide layer by HF solution. The lattice strain of the SiGe layer was evaluated by x-ray reciprocal-space maps obtained using a rotating anode x-ray generator.

Figure 1 shows the oxide thickness on the SiGe layer as a function of the oxidation time. The thickness of the oxide layer increases with the oxidation time for the $Si_{1-x}Ge_x$ (x=0–0.054) layers. We see that there is a tendency for the

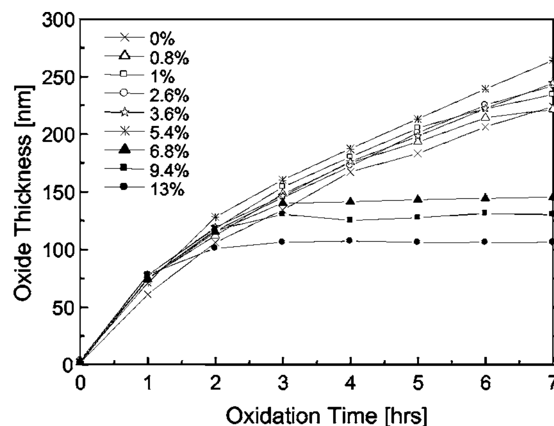

FIG. 1. Oxide thickness as a function of oxidation time. Ge concentrations in the initial SiGe alloy ranged from 0% to 13%. Oxidation temperature is 1000 °C.

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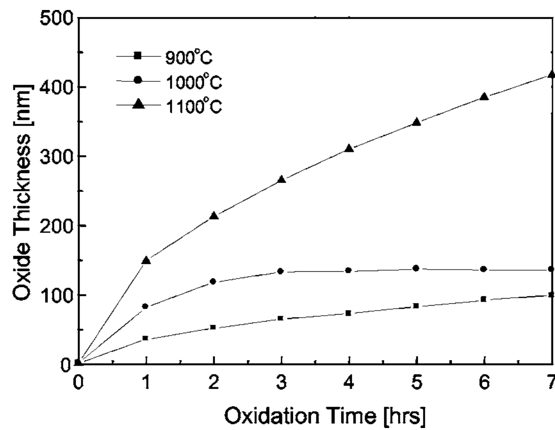

FIG. 2. Oxide thickness as a function of oxidation time. Ge concentration in the initial SiGe alloy is 12%. Oxidation temperatures ranged from 900 to 1000 °C.

oxidation rate to be higher for higher Ge concentrations in the initial SiGe alloy. This enhancement of the SiGe oxidation rate is in agreement with previous studies.[5] The oxidation rate does not increase with the oxidation time, although the Ge concentration of the SiGe layer increases. This is because the oxidation rate is limited by the diffusion of oxygen through the thick surface oxide layers. A characteristic feature in this figure is that oxidation stopped completely in the $Si_{1-x}Ge_x$ (x=0.068–0.13) layers after a few hours. For higher Ge concentrations, oxidation saturates after a shorter time, resulting in a thinner oxide layer.

In Fig. 2 the effect of the oxidation temperature on the oxidation rate is shown for the SiGe alloy having an initial Ge concentration of 12%. As the oxidation temperature increases, the oxidation rate increases during the initial stage of oxidation. Saturation of oxidation occurs for the sample oxidized at 1000 °C as Fig. 1 shows. Note that the thickness of the oxide layer for the sample oxidized at 1100 °C continues to increase after 7 h, even though its thickness is much greater than the saturation thickness of the sample oxidized at 1000 °C. In addition, oxidation saturation was not observed for the sample oxidized at 900 °C even after 7 h.

In order to clarify the mechanism for this self-limiting oxidation it is important to investigate the depth profile of the Ge concentration. Figure 3 shows the depth profiles of the Ge concentrations in the SiGe layers oxidized for 0, 1, 4, and 7 h. The depth is estimated by converting the etching time of Ar^+ sputter into depth on the basis of the thickness of the SiGe layers measured by ellipsometry; the position of the BOX layer is estimated by the depth profile of the O concentration. Figure 3(a) shows the results for a sample having an initial Ge concentration of 5.1%. We see that Ge atoms accumulate under the oxidized interface and diffuse into the SOI layer with increasing oxidation time. The total amount of Ge atoms remains constant within the accuracy of the measurement, indicating that the Ge atoms condense into the SiGe layer without Ge atoms being incorporated into the oxide layer.

In Fig. 3(b) the Ge concentration depth profiles are shown for the samples oxidized for 0–7 h having an initial Ge concentration of 16%. It is surprising that the profile for the sample oxidized for 7 h is almost the same as that for the sample oxidized for 4 h, even though it was oxidized at 1000 °C for an additional 3 h. A characteristic feature is the

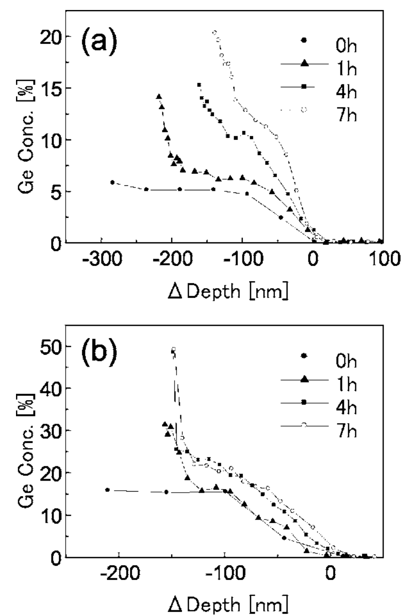

FIG. 3. Depth profiles of Ge concentration in SiGe layers oxidized for 0, 1, 4, and 7 h. The initial concentrations of Ge in the SiGe layers are 5.1% for (a) and 16% for (b). The interface between the SiGe and BOX layers is located at ΔDepth=0 nm.

abrupt increase below the top interface of the SiGe layers. It was also found by angle-resolved XPS measurement that the Ge concentration of the interfacial layer is 80% or greater, indicating the existence of a very thin layer, a few nanometers thick, with a Ge concentration of 80% or higher. These results indicate that the diffusion of Ge atoms just below the oxide layer is suppressed as well as the oxidation reaction of the SiGe alloy being suppressed.

X-ray reciprocal-space maps around the 113 Bragg point were obtained from the $Si_{1-x}Ge_x$ (x=0.16) samples. The reflection of the as-grown sample is observed close to the line of H, K=1.00, indicating that the SiGe layer is pseudomorphic. However, the position of the reflection of the SiGe layer oxidized for 4 h indicates that the strain in the SiGe layer is almost relaxed. The peak of the SiGe layer is weak and broad, showing that the crystalline quality of this layer is poor.

The diffusion coefficient of Ge in SiGe alloy depends on the Ge concentration. The coefficients at 1000 °C were reported to be 1.08×10^{-16}–1.03×10^{-15} in Si and 1.21×10^{-13} cm^2/s in $Si_{0.776}Ge_{0.224}$.[7–10] The respective diffusion lengths are 6–19 and 209 nm/h. It is clear that the suppres-

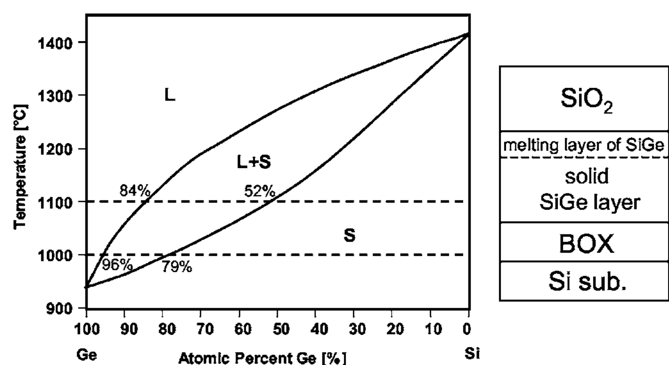

FIG. 4. Phase diagram of Si–Ge system (Ref. 11) and a schematic drawing of the melting layer for the saturated SiGe layer.

sion of the diffusion of Ge atoms just below the surface oxide layer cannot be explained by a diffusion mechanism based on the concentration gradient.

Tezuka *et al.* proposed that the strain in the SiGe layer is one possible reason for the reduction in the oxidation rate of the SiGe layer on the basis of measurements of the residual strain in SGOI layers by Raman spectroscopy.[1] The strain in SiGe, arising from the gradient of the Ge fraction, suppresses the diffusion of Si to the oxidized interface through the SiGe layer. However, we found that the strain in the SiGe layer oxidized for 4 h was almost relaxed for the $Si_{1-x}Ge_x$ ($x=0.16$) sample using x-ray reciprocal-space map technique, indicating that the oxidation stops for the sample where there is no strain in the SiGe layer. This means that the self-limiting oxidation is not due to lattice strain in the SiGe layer.

Instead, we propose a model in which the self-limiting oxidation is due to the melting of an interfacial layer having a high Ge concentration between the surface oxide and the SiGe layers (Fig. 4). As the oxidation time increases, Ge concentration just below the surface oxide layer increases. According to the phase diagram for the Si–Ge system,[11] the interfacial layer melts when the concentration becomes more than 79% for the oxidation at 1000 °C. The interfacial layer consists of a mixture of liquid and solid phases having Ge concentrations of 96% and 79%, respectively. If it is assumed that the mixed layer separates into liquid and solid layers to reduce the interfacial free energy between the liquid and solid phases and that the liquid layer is adjacent to the oxidized interface, then the oxidation rate would rapidly decrease, since the Si concentration is just 4% at the oxidized interface. The diffusion of Ge atoms would also be suppressed because the liquid and solid layers are stable at 1000 °C.

Saturation of oxidation is not observed for the sample oxidized at 1100 °C, even though the interfacial layer melts. In this case the Si concentration of the liquid layer covering the oxidized interface is 16%, which is four times higher than that for the oxidation carried out at 1000 °C. This is the reason why oxidation is not saturated at 1100 °C. Saturation is not expected for oxidation at 900 °C, because this temperature is below the melting point of pure Ge.

In conclusion, we have experimentally demonstrated the phenomenon of self-limiting oxidation of SiGe alloy. For oxidation at 1000 °C, oxidation stopped completely after a few hours of oxidation of the $Si_{1-x}Ge_x$ ($x=0.068-0.16$) layers. For higher initial concentrations of Ge in the SiGe layer, the oxidation saturated in a shorter time. Saturation was not observed for the oxidation at 900 and 1100 °C. To explain these results we propose a model in which the self-limiting oxidation is caused by melting of an interfacial layer having a high Ge concentration.

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