

## Temperature Dependence of Exclusive SiO<sub>2</sub> Formation during Thermal Oxidation of Si<sub>1-x</sub>Ge<sub>x</sub> Alloy Layer on Si(001) Surfaces

Hideaki Hozumi<sup>1</sup>, Shuichi Ogawa<sup>1</sup>, Akitaka Yoshigoe<sup>2</sup>, Shinji Ishidzuka<sup>3</sup>, James R. Harries<sup>2</sup>, Yuden Teraoka<sup>2</sup>, and Yuji Takakuwa<sup>1</sup>

<sup>1</sup>Tohoku Univ., Institute of Multidisciplinary Research for Advanced Materials, 2-1-1 Katahira, Aoba-ku, Sendai, Miyagi 980-8577, Japan

Phone: +81-22-217-5367 E-mail: hozumi@mail.tagen.tohoku.ac.jp

<sup>2</sup>Japan Atomic Energy Agency, Quantum Beam Science Directorate, 1-1-1 Koto, Sayo-cho, Sayo-gun, Hyogo 679-5198, Japan

<sup>3</sup>Akita Nat. Col. Tech, Dept of Applied Chemistry, 1-1 Iijimabunkyo-cho, Akita, Akita 011-8511, Japan

### 1. Introduction

A strained Si channel and high k gate stack has been developed for next generation complementary metal-oxide-semiconductor (CMOS) devices. Particularly the strained Si channel is available for high-speed operation of LSI by enhancing the carrier mobility. Such a channel is typically formed on a strain-relaxed Si<sub>1-x</sub>Ge<sub>x</sub> alloy layers with the oxidation-induced Ge condensation process. Recently, it was reported that the Si<sub>1-x</sub>C<sub>x</sub> or Si<sub>1-x</sub>Ge<sub>x</sub> alloy layers are directly used as the strained channel [1]. Therefore, the clarification of the concentration mechanism of Ge atoms for gate stack formation is very important. It was reported that the oxidation rate of Si<sub>1-x</sub>Ge<sub>x</sub> alloy layers is faster than that of a Si(001) surface [2] and Ge atoms do not oxidized and diffuse into SiO<sub>2</sub>/SiGe interface [3]. In this study, the oxidation reaction kinetics on the Si<sub>1-x</sub>Ge<sub>x</sub> alloy layer was investigated by real-time X-ray photoelectron spectroscopy (XPS) to reveal the oxidation states of Ge that is doped for strain-control and the effect of strain on oxidation reaction kinetics. In addition, temperature dependence of Ge condensation kinetics due to oxidation is clarified by analyzing the time evolution of Ge 3d intensity.

### 2. Experiments

Experiments were performed using the surface reaction analysis apparatus (SUREAC2000) installed at the BL23SU of SPring-8, Japan. In this experiment, a p-type Si(001) was used as the substrate. The Si substrate was cleaned with annealing in ultra-high-vacuum. After cleaning, Ge is deposited on to the Si(001) surface at room temperature (RT) and then the surface was annealed at 660°C for 20 min. The Ge atoms diffused into the Si substrate due to dimerization stress and then Si<sub>1-x</sub>Ge<sub>x</sub> alloy layer was formed during annealing. The Si<sub>1-x</sub>Ge<sub>x</sub> alloy layer was oxidized at RT or 500°C. The dry O<sub>2</sub> gas of 99.995% purity was introduced into reaction chamber up to  $5.0 \times 10^{-5}$  Pa during 5300 s. In order to enhance the oxidation reaction, the O<sub>2</sub> pressure was increased up to  $1.3 \times 10^{-3}$  Pa and the substrate was oxidized for 6400 s. During oxidation, the O 1s, Si 2p and Ge 3d photoelectron spectra were measured alternately for 5, 63 and 52 s. The photon energy and detection angle were 709 eV and 70°, respectively.

### 3. Results and discussion

The Ge coverage was estimated from the photoelectron intensity ratio of Ge 3d to Si 2p. It is found that the Ge coverage before oxidation is approximately 1.5ML and 2.5ML at RT and 500°C, respectively. Figure 1 shows the time evolution of O 1s photoelectron intensities at (a) RT and (b) 500°C on the Si and SiGe surfaces. O 1s intensities rapidly increase until 2000 s, and then gradually increase at both temperatures. In Fig. 1 (a), oxidation rate on the SiGe alloy surface is slower than that of the Si(001) surface. O 1s uptake on the SiGe surface at 500°C also increases slower than that on the Si(001) surface in Fig. 1.(b). These results indicate that the Ge mixture prevents the oxide film growth. Figure 2. shows the Si 2p<sub>3/2</sub> photoelectron spectra on the

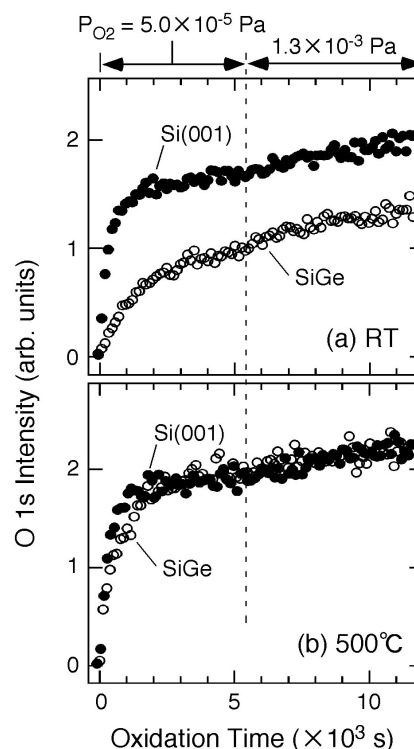


Fig. 1. Time evolution of O 1s photoelectron intensities at (a) RT and (b) 500°C on the Si(001) surface (open circles) and the SiGe alloy surface (closed circles).

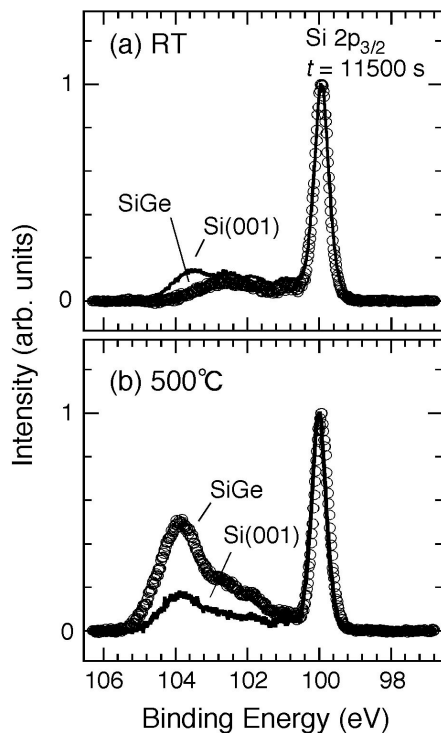


Fig. 2. Si  $2p_{3/2}$  photoelectron spectra on SiGe (open circles) and Si(001) surface (solid line) at the end of oxidation at (a) RT and (b) 500°C. These spectra are normalized by Si  $2p_{3/2}$  bulk intensities each.

SiGe and Si(001) surfaces at the end of oxidation at (a) RT and (b) 500°C. These spectra are normalized by Si  $2p_{3/2}$  bulk intensities to compare the oxide components with each other. In Fig. 2.(a), the  $Si^{4+}$  component on the SiGe alloy surface is less than that on the Si(001) surface, so it is found that the  $SiO_2$  films do not grow at RT. However,  $Si^{4+}$  component at 500°C grows more than that at RT in Fig. 2.(b). Figure 3. shows the temperature dependence of Ge 3d photoelectron spectra at the end of oxidation ( $t = 11700$  s) between RT and 500°C. These spectra are normalized by

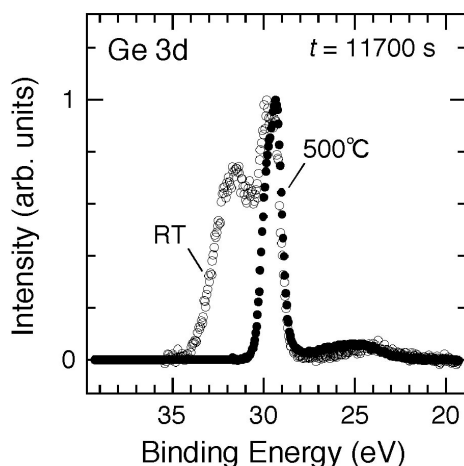


Fig. 3. Temperature dependence between RT (open circles) and 500°C (closed circles) of Ge 3d photoelectron spectra at the end of oxidation. These spectra are normalized by Ge 3d Si-Ge bonding component intensities.

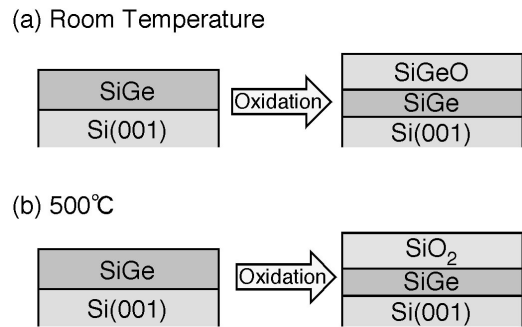


Fig. 4. Schematic illustration of the structural model of the oxidized SiGe alloy surfaces at (a) RT and (b) 500°C

Ge 3d intensity (Si-Ge bonding component). It is clear in Fig. 3 that the Ge atoms are oxidized at RT whereas no Ge oxidation occurs at 500°C.

Above all, it is clarified that the no Ge atoms on the SiGe alloy surface are oxidized and Si atoms are oxidized preferentially. The Ge atoms diffuse into the substrate well known as the oxidation condensation of Ge. The Ge diffusion is not caused due to thermal diffusion because the oxidation temperature of 500°C is sufficiently low in comparison to annealing at 660°C. The diffusion of Ge was not enhanced during annealing. Therefore, it is suggested that the diffusion of Ge is caused by the point defect generation due to oxidation-induced strain [4]. On the other hand, the diffusion does not occur at RT because Ge oxide component clearly appears in Fig. 3. In addition, oxidation rate on SiGe alloy surface is less than that on Si(001) surface. It can be assumed in unified oxidation reaction model [4] that the slow oxidation rate indicates less generation of the defects, thus the diffusion of Ge does not occur at RT. The structural models of the oxidized SiGe alloy surfaces at RT and 500°C are summarized in Fig. 4. It is found that the condensation of Ge needs oxidation at temperatures more than 500°C.

#### 4. Conclusions

In order to clarify the concentration mechanism of Ge atoms for strained-Si CMOS devices, the oxidation reaction kinetics of  $Si_{1-x}Ge_x$  alloy layer was observed by real-time XPS. By comparison of the oxidation reaction kinetics on the  $Si_{1-x}Ge_x$  alloy layer among two oxidation temperature (RT and 500°C), it was found that Ge was significantly oxidized at RT, although  $SiO_2$  was exclusively formed at 500°C. This result indicates that the oxidation rate of Ge atoms depends of the diffusion of Ge atoms due to oxidation-induced strain.

#### References

- [1] Y.C. Yeo, *Semicond. Sci. Technol.* **22** (227) S177.
- [2] H. Nohira, *et al.*, *Appl. Surf. Sci.* **237** (2004) 134.
- [3] M. Spadafora, *et al.*, *Appl. Phys. Lett.* **83** (2003) 3713.
- [4] S. Ogawa and Y. Takakuwa, *Jpn. J. Appl. Phys.* **46** (2006) 7063.