Time-Dependent Selective Oxidation by Low Pressure Oxidation on High-Ge-Content SiGe

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Abstract

In this study, low-pressure oxidation (LPO) process has been used to form the passivation layer on high-Ge-content (HGC) Si_{0.16}Ge_{0.84} surface. X-ray photoelectron spectra of the oxide layer showed that with an increase in oxidation time, the mixed oxide (SiO_x + GeO_x) was detected. The oxide growth rate after 5 min was limited by the diffusion of oxidant due to the formation of mixed oxide. Finally, the optimization of oxidation time for LPO process was used to demonstrate the HGC SiGe MOSCAP with EOT = 1.2 nm and interface trap density (D_{it}) value of $1 \times 10^{12} \text{ eV}^{-1} \text{cm}^{-2}$.

1. Introduction

HGC SiGe has received more attentions for 5 nm node and beyond logic appilcation due to the enhancement of hole mobility from its material characteristic, together with built-in compressive strain from global buried SiGe SRB stressor [1]. However, high interface quality between high- κ dielectrics and the HGC SiGe channel remain challenging since volatile species GeO_x tend to form and desorb during subsequent annealing, thus enhancing the D_{it} in the bandgap. Although low-pressure oxidation (LPO) has been demonstrated to be able to form high SiO_x composition with low GeO_x composition in the IL on SiGe surface [2], the detailed oxidation mechanism still remains ambiguous.

In this study, we conducted the LPO process on HGC SiGe with various oxidation time and presented a series of material analyses to elucidate the effect of the LPO process on atomic diffusion behavior.

2. Experiment

HGC Si_xGe_{1-x} layer on relaxed Ge buffer layer was grown on p-type Si (100) substrate by LPCVD system. From the XRD and RSM analyses shown in **Fig. 1**, the thickness and the Ge content of the SiGe layer was 40 nm and 84%, respectively, fitting from the Pendellosung fringes of 2θ - ω scans. The LPO process was conducted at the same oxidation temperature and pressure (600 °C/0.01 torr) for 5, 10, 20, 40 min, after the native oxides on SiGe wafer were removed using diluted HF and DI water. Then, XPS with Ar⁺ ion beam was used to characterize the bonding states of Ge 3d and Si 2p and their intensity as a function of depth. For the fabrication of MOSCAP, 40-cycles HfO₂ was deposited through plasma-enhanced ALD and subsequently post-deposition annealing (PDA) in N₂ ambient was performed at 500 $^{\circ}$ C for 1 min. Finally, a 50-nm TiN gate was sputtered, followed by deposition of Ti/Al as the backside contact.

3. Results and Discussion

Figures 2 present the XPS elemental depth profile of Ge 3d and Si 2p core levels after the LPO process. During the first 5 min of oxidation, the growth of GeOx was effectively suppressed and only SiOx was formed. However, as the oxidation time was extended from 5 to 20 min, the intensity of both Ge-O and Si-O significantly increased, indicating the formation of the mixed oxide layer (SiO_x + GeO_x). Moreover, GeO_x showed higher intensity close to the surface of oxide layer. Fig. 3. shows the separated XPS signals of GeO_x, SiO_x, Ge, and Si composition profile by using the peak area and relative sensitivity factor. As the etching time of 20 min case increased to 180 s, a Ge-rich layer was present which located below the oxide layer. Fig. 4 shows the measured oxide thickness by XRR as a function of time. The LPO process followed a parabolic regime, indicating the growth rate was limited by the diffusion of oxidant through existing oxide, however, which is in contradiction with Deal and Grove model for thin oxides.

Figures 5 show the speculated schematic illustration of LPO process on HGC SiGe substrate. At initial oxidation stage, Si was preferentially oxidized in low oxidation pressure condition based on the principle of thermodynamics, which resulting in the Si from SiGe substrate self-diffused toward the oxidizing interface. However, as the Si depleted layer became larger than Si self-diffusion length and formed Ge-rich layer, the reaction between pure Ge and oxidant occurred until the oxidation front reached a region where Si could be provided. During this long period of alternation of Si and Ge oxidations, a mixed oxide formed and the interfacial oxygen concentration decreased with increasing oxide thicknesses, leading to a decrease of the oxidation rate, which could explain the result shown in Fig. 4. Therefore, the rate-limiting step of LPO process performed from 5 to 40 min was the diffusion of oxidant through the increasing mixed oxide layer.

In view of suppression of GeO_x formation and EOT scaling, the LPO process was performed for 3 min on HGC SiGe substrate. **Fig. 6** shows the multi-frequency Capacitance-Voltage (C-V) characteristics of the TiN/HfO₂/IL/SiGe before and after series resistance

correction. The frequency dispersion effects of C-V curve in accumulation originated from series resistances of the undoped Ge buffer layer. The corresponding D_{it} distributions extracted by two band admittance circuit model [3] and conventional conductance method are shown in **Fig.** 7. Without the minority carrier response, the lowest D_{it} value of $1 \times 10^{12} \text{ eV}^{-1} \text{ cm}^{-2}$ near E-E_v = 0.13 eV was achieved for the LPO process.

4. Conclusions

We investigated the oxidation behavior of Si_{0.16}Ge_{0.84} by LPO process. The XPS spectra showed that the elongation of the oxidation time led to the mixed oxide formation. In order to allow Si to be preferentially oxidized, it is necessary to control the oxidation time in addition to operating at a low pressure environment. HGC SiGe MOSCAP with nearly GeO_x-free IL showed the lowest D_{it} value (1×10¹² $eV^{-1}cm^{-2}$) with the correction of series resistance and minority carrier response.

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References

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Fig. 1 (a) XRD spectra and (b) RSM for the HGC Si_xGe_{1-x} layer grown on relaxed Ge layer.



Fig. 2 XPS element depth profile of (a) Si 2p, (b) Ge 3d using LPO

to 5, 20 min and the red dash line indicated the signals of oxide and SiGe substrate.



Fig. 3 XPS signals of GeO_x , SiO_x, Ge, and Si composition profile of LPO 5 min and 20 min, the black dash line indicated the interface between oxide and SiGe.



Fig. 4 Oxide thickness as a function of the oxidation time for LPO process on SiGe substrate.









Fig. 7 D_{it} distributions were extracted based on the two band circuit model [3] and conductance method.