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Effects of Oxynitride-Based Interface Control on HfO_2 MIS Properties and FET Performance

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1. Introduction

Control of high-k/Si interface is a key factor to obtain the robust structure for sub-100nm high-k gate CMOS. Recently, nitride-based interface control was applied to form thermally stable interfaces between high-k and Si[1,2]. However, the influence of oxynitride-based (including nitride-based) interface control on electrical properties of MIS structures has not been studied systematically.

In this paper, electrical properties of the HfO_2 MIS structures with the oxynitride-based interfaces prepared by various processes are examined under the fixed HfO_2 deposition and post-deposition processes.

2. Experimental Procedure

Various interface control (see Table I) on *p*-type Si (100) (resistivity 1-5 Ωcm) substrates was performed immediately after removing the chemical oxide layer formed by a conventional RCA cleaning. The composition and the physical thickness of prepared interface-control layers (ICLs) were measured using Auger electron spectroscopy (AES). The dielectric constant k of the interface oxynitride layer was evaluated using an experimental relationship between x and k, where x was defined as $(SiO_2)_x(Si_3N_4)_{1-x}$ for the SiON system [3].

2 nm-thick HfO_2 films were deposited onto ICLs at 200 °C by KrF excimer laser ablation in 0.1 Torr N_2 ambient, followed by 15 s RTA in a N_2 atmosphere (>99.99995 % purity) at 800°C. Au electrodes (200μm in diameter) and Al were deposited onto the HfO_2 films and the backside of the substrates, respectively.

3. Results and Discussion

We first discuss leakage current, then we describe influence of nitrogen density in ICLs on equivalent oxide thickness (EOT), flat-band voltage V_{FB}, and V_{FB} hysteresis of the HfO_2 MIS structures, as well as performance of FETs.

Figure 1 shows the leakage current (J_g) versus EOT of the HfO_2 MIS structures with various interface control. EOT was extracted from the comparison between measured *C-V* curves and ideal *C-V* curves [4]. For all the samples, Jg values are several orders magnitude lower than those of SiO_2 [5].

Figure 2 shows EOT of the HfO_2 MIS structures versus nitrogen density (N_N) in the ICLs. The results show a clear trend that the process induced EOT increase is suppressed with increasing N_N, though a process dependent variation can still been seen. From this plot, $N_N \approx 4\times10^{15}cm^{-2}$ is considered to be the minimum N_N to prevent the EOT for the sample structure and RTA condition described above. TEM observation also supports that the ICLs with higher nitrogen than this value are thermally stable in the RTA process (Fig. 3).

We have also found that V_{FB} is linearly reduced with N_N (Fig. 4). We estimated the fixed charge densities in the interfacial layer (N^{fix}_{int}) and the HfO_2 layer (N^{fix}_{HfO2}), under the assumption that distribution of the fixed charges in each of these layers is uniform. As a result, the interface fixed charge $N^{fix}_{int} = \alpha N_N$ (positive, $\alpha = 1.8\times10^{-3}$) and the HfO_2 fixed charge $N^{fix}_{HfO2} = 7.5\times10^{13}$ cm^{-2} (negative) were obtained.

Furthermore, the result shown in Fig. 5 indicates that the flat-band voltage hysteresis V_{hys} changes with N_N. This fact suggests that the contribution of carrier-injection from the substrate to V_{hys} might become larger than that from the Au electrode with the increase of surface nitrogen density N_N.

Based on the experimental results, we now discuss the impact of ICLs on the performance of the HfO_2 MISFETs as shown in Fig. 6. As a figure-of-merit for the current-drivability of the MISFETs, we introduce μ_{eff}/CET_{gate}. Here, μ_{eff} and CET_{gate} are the effective mobility and capacitance equivalent thickness of the gate stack, respectively. We estimate the optimum composition x of ICL at N_N=$4\times10^{15}cm^{-2}$ according to the following procedures.

First, CET_{gate} was estimated as $CET_{gate} = EOT_{ICL} + EOT_{HfO2} + EOT_{inv}$, where the 2nd and 3rd terms are EOT of HfO_2 and inversion layer [6], respectively. As shown in Fig. 7, EOT of the oxynitride layer (EOT_{ICL}) varies along the bold curve by changing x. Second, the mobility degradation was calculated by taking account of the remote charge scattering [7] from the fixed charges both from ICL and HfO_2. Figure 8 shows the calculated μ_{eff} and μ_{eff}/CET_{gate} as a function of SiO_2 composition x in ICL at N_N=$4\times10^{15}cm^{-2}$. With x decrease, the calculated μ_{eff} significantly decreases because of physical proximity of fixed charges in ICL and HfO_2 to the Si interface. Although μ_{eff}/CET_{gate} is determined by the competing effects of mobility degradation and increase of $1/CET_{gate}$ with decreasing of x, the result in Fig. 8 indicates that it has the maximum value at x = 0.

Figure 7 shows that EOT_{ICL} at x = 0 (and $N_N = 4\times10^{15}$ cm^{-2}) is 0.4 nm. This EOT corresponds to the physical thickness of 0.76 nm (about 2 monolayer (ML) of Si_3N_4). Thus, below 2 ML Si_3N_4, it is difficult to suppress the surface reaction, while above 2ML Si_3N_4, EOT_{ICL} increases due to the increase of the Si_3N_4 thickness itself. This result suggests that the interface with about 2 ML Si_3N_4 is effective for obtaining the optimum FET performance.

4. Conclusions

We have performed a series of experiments in which both interface nitridation method and nitrogen density have been changed in HfO_2 MIS capacitors. We have found that EOT, V_{FB}, and V_{hys} of the HfO_2 MIS structures vary systematically with the sheet density of nitrogen in as-prepared ICLs. By using the experimentally obtained N_N criterion, the optimum performance of HfO_2 MISFET has been expected in the interface layer with about 2ML of Si_3N_4.

Acknowledgments

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References

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Table I Interface control layers (ICLs) examined and their preparation method.

ICL (T_{phy})	Process	Marker
Hydrogen-terminated	HF-last	⧓
SiO_2 (0.5-0.6nm)	Annealing in O_2 UV irradiation in O_2	▲ △
Oxynitride (0.4-1.1nm)	Annealing in NO Remote plasma(N_2/He) Direct plasma (N_2/He)	◆ □ ■
Nitride (0.4-1.5nm)	Annealing in NH_3 RF nitrogen radical	● ○

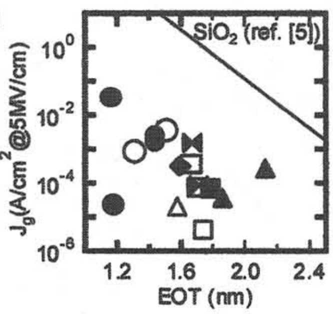


Fig. 1 The leakage current J_g versus EOT of the HfO_2 MIS structures with various interface control layers.

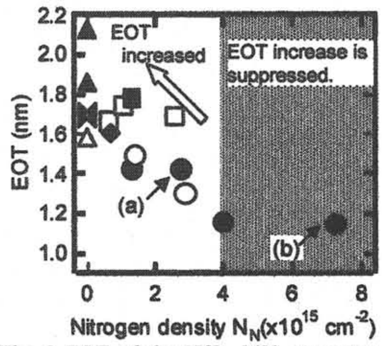
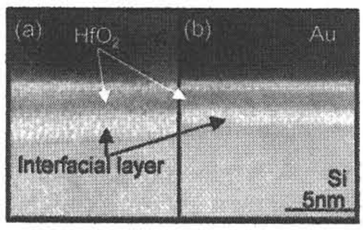


Fig. 2 EOT of the HfO_2 MIS structures with various interface control layers is plotted as a function of N_N. Cross-sectional TEM images of sample (a) and (b) are shown in Fig. 3.



N_N =2.7x10^{15} cm^{-2} N_N =7.2x10^{15} cm^{-2}

Fig. 3 The cross-sectional TEM images for the samples after RTA at 800°C. (a) and (b) correspond to the sample (a) and (b) in Fig.2, respectively. (a): The interfacial layer is much thicker than that of the initial ICL. (b): Thickness of the interfacial layer is almost the same as that of the initial ICL. Note that HfO_2 thickness is unchanged for both cases after RTA.

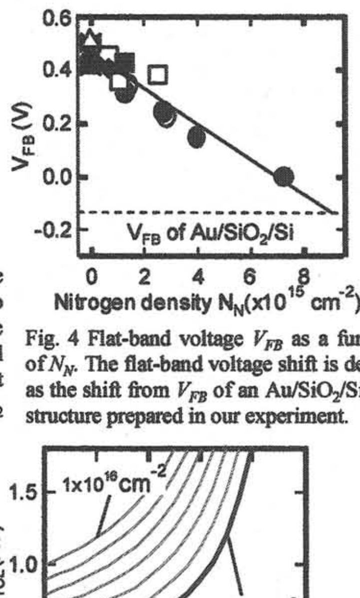


Fig. 4 Flat-band voltage V_{FB} as a function of N_N. The flat-band voltage shift is defined as the shift from V_{FB} of an Au/SiO$_2$/Si MIS structure prepared in our experiment.

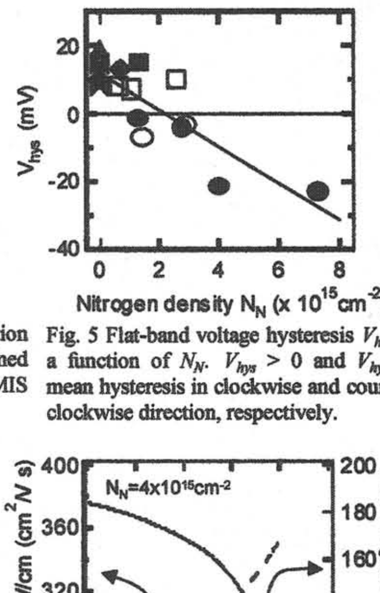


Fig. 5 Flat-band voltage hysteresis V_{hys} as a function of N_N. V_{hys} > 0 and V_{hys} <0 mean hysteresis in clockwise and counter-clockwise direction, respectively.

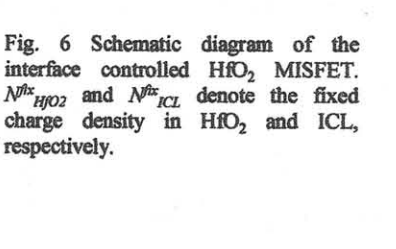


Fig. 6 Schematic diagram of the interface controlled HfO_2 MISFET. N^{fix}_{HfO2} and N^{fix}_{ICL} denote the fixed charge density in HfO_2 and ICL, respectively.

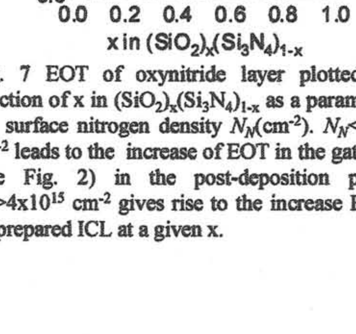


Fig. 7 EOT of oxynitride layer plotted as a function of x in $(SiO_2)_x(Si_3N_4)_{1-x}$ as a parameter of the surface nitrogen density N_N(cm^{-2}). N_N<4x10^{15} cm^{-2} leads to the increase of EOT in the gate stack (see Fig. 2) in the post-deposition process. N_N>4x10^{15} cm^{-2} gives rise to the increase EOT of as-prepared ICL at a given x.

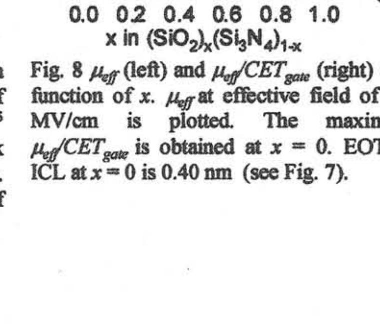


Fig. 8 μ_{eff} (left) and μ_{eff}/CET_{gate} (right) as a function of x. μ_{eff} at effective field of 0.4 MV/cm is plotted. The maximum μ_{eff}/CET_{gate} is obtained at x = 0. EOT of ICL at x = 0 is 0.40 nm (see Fig. 7).