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Influence of Post Cap-layer Deposition Annealing Temperature on MgO Diffusion in High-k/IFL Stacks

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Introduction

Metal gate/dual high-k CMISFETs have attracted much attention to achieve low V_t CMISFETs with scaled EOTs [1-2]. Recently, Mg incorporated high-k dielectrics have been found to be attractive for V_t reduction of nMISFETs [3-5]. However the extent of V_t reduction induced by Mg incorporation varied with the reported device fabrication process. Thus then, details of relationship between fabrication process and V_t reduction by Mg incorporation must be understood for optimization of the fabrication process of Mg incorporated high-k dielectrics. Therefore, we have investigated the flatband voltage (V_{fb}) shift dependence on device fabrication process.

Device Fabrication

Fig. 1 shows the sample fabrication process employed in this study. After IFL formation, HfO_2 was deposited as the base high-k dielectric using atomic layer deposition (ALD) technique and post deposition annealing (PDA) was performed at 850 ºC. Next, Mg was deposited with a physical vapor deposition (PVD) technique and a subsequent oxidation in an O_2 ambient at R.T. was performed. After this MgO deposition, post cap-layer deposition annealing (PCA), was applied at several temperatures for 5 seconds in an N_2 ambient. Then, TiN and poly-Si were deposited using PVD and CVD technique, respectively. After gate electrodes ware formed by dry etching, extension and source/drain region were formed by ion implant and spike RTA at 1000ºC. EOT and V_{fb} are extracted using "MIRAI-ACCEPT" [6].

Results and Discussion

Mg thickness dependence (PCA temperature 1050 ºC)

Fig. 2 shows CV curves of HfO_2 and MgO incorporated HfO_2 (MgO/HfO_2), with several thickness of MgO, where the PCA was performed at 1050 ºC. The thickness of SiON-IFL and HfO_2 were 0.7 nm and 2.0 nm, respectively. The thicknesses of Mg were 0.18, 0.30, and 0.42 nm. The CV curves of MgO/HfO_2 are slightly shifted from that of HfO_2. Fig. 3 shows the relationship between Mg thickness and V_{fb} extracted from fig. 2. V_{fb} of MgO incorporated HfO_2 is shifted in the negative direction, but this shift is slight. Moreover, the V_{fb} shift is independent of the MgO thickness. To investigate in more detail, Mg profiles in MgO incorporated HfO_2 were evaluated by Secondary Ion-microprobe Mass Spectrometry (SIMS). Fig. 4 shows back-side SIMS depth profiles of MgO incorporated HfO_2 stacks, where the Mg thicknesses were 0.3 and 0.42 nm. It clearly shows that, after 1050 ºC PCA, the amount of Mg in the MgO incorporated HfO_2 is almost same, even though the deposition thicknesses were different.

PCA temperature dependence (Mg thickness 0.3-nm)

Fig. 5 shows CV curves of HfO_2 and MgO incorporated HfO_2 with PCA at several temperatures. The thickness of SiON-IFL, HfO_2, and Mg were 0.7 nm, 2.0 nm and 0.3 nm, respectively. The temperatures of PCA were 800, 950, 1000, and 1050 ºC. Fig. 6 shows relationship between PCA temperature and V_{fb}, extracted from fig. 5. By decreasing the PCA temperature, V_{fb} of MgO incorporated HfO_2 is greatly shifted to the negative direction. Fig. 7 shows back-side SIMS depth profiles in MgO incorporated HfO_2 for several PCA temperatures. It clearly shows that the amount of Mg in MgO incorporated HfO_2 decreases with increasing PCA temperature. This indicates that the differences in V_{fb} shift in fig. 6 reflect the difference in concentration of Mg in the MgO incorporated HfO_2.

Comparison between on SiO_2 and on HfO_2

To understand the mechanism of the decrease in Mg concentration with high temperature PCA, we investigated the thermal stability of MgO on SiO_2 and HfO_2. Fig. 8 shows the area density of Mg atoms after MgO deposition and PCA on SiO_2 or HfO_2/SiO_2, as evaluated by X-ray Fluorescence Analysis. The temperatures of the PCA were 850 or 1050 ºC. The thickness of Mg, SiO_2, HfO_2, and SiO_2-IFL were 0.42 nm, 100 nm, 2.8 nm, and 0.8 nm, respectively. In case of deposition on SiO_2, Mg atoms were not much reduced. On the other hand, in case of deposition on HfO_2/SiO_2, Mg atoms were decreased massively to the value less than 5.0×10^{12} atoms/cm^2 after 1050 ºC PCA. Fig. 9 shows the O *1s* photoelectron spectra of MgO/SiO_2, before and after thermal annealing at 900 ºC. After annealing, Mg-O bonds were reduced, and Si-O peak was shifted between the Si-O and Mg-O bond energy positions. It is thought that $MgSiO_x$ had been generated as MgO reacted with SiO_2 after annealing. From these results, it is supposed that the decrease in Mg concentration during PCA is accelerated with HfO_2 and Mg can remain in the SiO_2, forming Mg silicate.

IFL thickness dependence (PCA temperature 1050 ºC)

Fig. 10 shows the EOT-V_{fb} plot for HfO_2 and MgO incorporated HfO_2. The thicknesses of HfO_2 and Mg were 2.0 nm and 0.3 nm, respectively. The thicknesses of SiO_2-IFL were 0.8, 1.2, and 4.0 nm. The temperature of PCA was 1050 ºC. In case of HfO_2 without MgO incorporation, V_{fb} dependence on IFL thickness was small. With MgO incorporation, the extent to which V_{fb} shifted towards the negative direction increased with increasing the SiO_2-IFL thickness. Fig. 11 shows back-side SIMS depth profiles of MgO incorporated HfO_2 with several thicknesses of IFL. The amount of Mg increased according to the SiO_2-IFL thickness.

From results obtained in this work, we supposed a model for Mg concentration decrease in PCA as schematically shown in fig. 12. Most of MgO deposited on HfO_2/IFL was diffused to IFL and formed Mg silicate under the PCA conditions of relatively low temperature, such as 850 ºC. Under the high temperature environment, such as 1050 ºC, although MgO itself has very high temperature boiling point of 3600 ºC, Mg may diffuse out from HfO_2 or sublimate due to Mg or Mg^+ generation during diffusion in HfO_2.

Conclusion

The extent of V_{fb} shift by incorporating MgO into HfO_2/IFL gate dielectric with PCA depends strongly on both the PCA temperature and the IFL thickness. Low PCA temperature is required to achieve a large V_t reduction, maintaining a small EOT with thin IFL for the 32 nm node and beyond.

References

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[3] V. Narayanan et al., VLSI symp., p.178, 2006
[4] N. Mise et al., IEDM Tech. Dig., p.527, 2007
[5] S. Kamiyama et al., IEDM Tech Dig., p41, 2008
[6] N. Yasuda et al., Ext. Abst. SSDM Tech. Dig., p.250, 2005.

- STI formation
- IFL (SiON or SiO_2) formation
- HfO_2 deposition (2.0nm)
- PDA (850ºC)
- Mg deposition & Oxidation
- PCA (Post Cap-layer deposition anneal)
- PolySi/TiN deposition
- Gate formation
- Halo, SDE, SD I/I
- Spike RTA (1000ºC)

Fig.1 Sample fabrication flow.

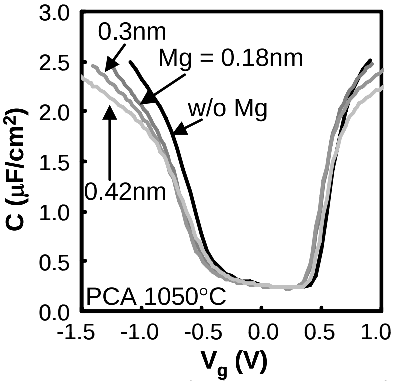

Fig. 2 CV curves of HfO_2 and MgO/HfO_2 with several thickness of MgO. The PCA was performed at 1050 ºC

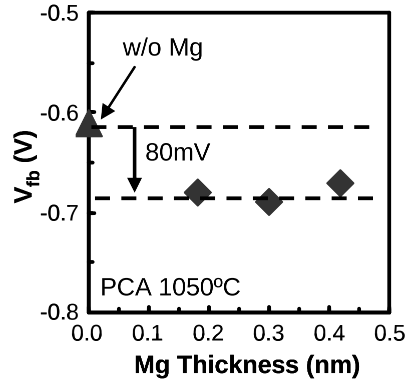

Fig. 3 Relationship between Mg thickness and V_{fb}. The V_{fb} shift is slightly, moreover, it is independent of Mg thickness.

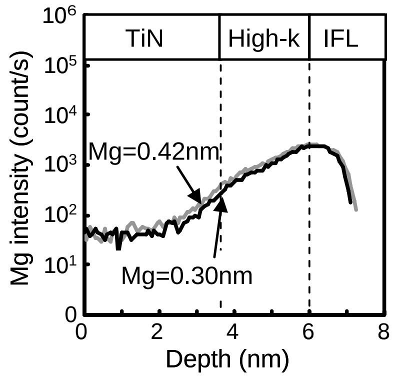

Fig. 4 Backside SIMS profiles of MgO/HfO_2. after 1050 ºC PCA, the amount of Mg is almost the same.

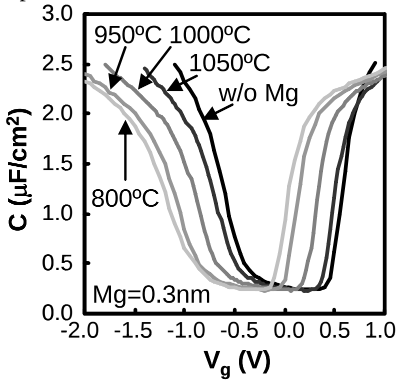

Fig. 5 CV curves of HfO2 and MgO/HfO_2 with PCA at several temperatures, where the thickness of Mg was 0.3nm.

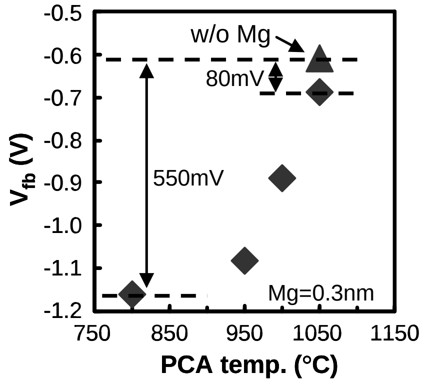

Fig. 6 Relationship between PCA temp. and V_{fb}. By decreasing PCA temperature, V_{fb} of MgO/HfO_2 is greatly shifted.

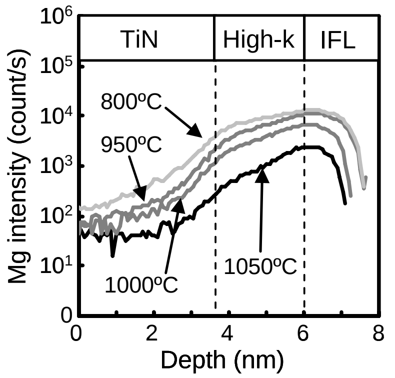

Fig. 7 Backside SIMS profiles of MgO/HfO_2. The amount of Mg decreases with increasing PCA temperature.

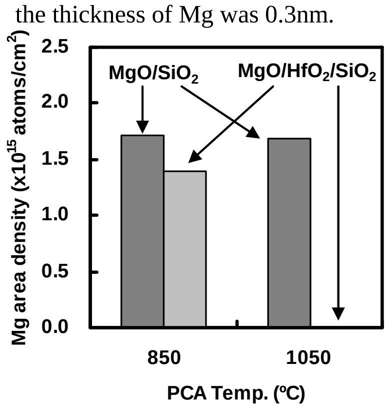

Fig. 8 The area density of Mg atoms on SiO_2 or HfO_2/SiO_2 after PCA evaluated by X-ray Fluorescence Analysis. Mg atoms are not decreased on SiO_2.

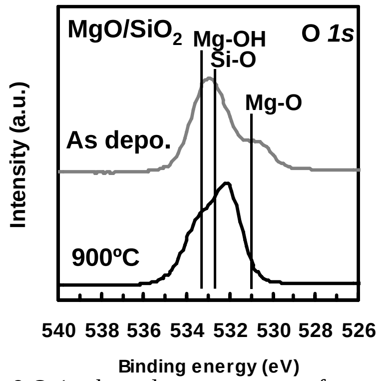

Fig. 9 O *1s* photoelectron spectra of MgO/SiO_2 before and after PCA at 900 ºC. After PCA, the peak located between Si-O and Mg-O is increased.

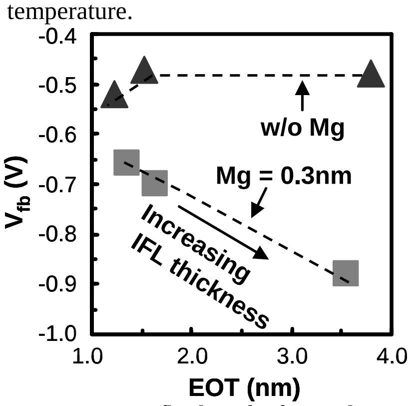

Fig.10 EOT-Vfb plot of HfO_2 and MgO/HfO_2 with several thickness of SiO2-IFL.

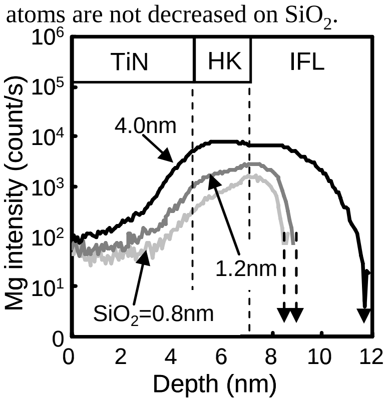

Fig.11 Backside SIMS profiles of MgO/HfO_2 with several thicknesses of SiO_2-IFL. The amount of Mg increases according to the SiO_2-IFL thickness.

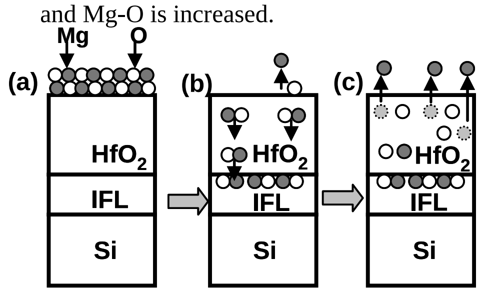

Fig.12 Schematics of supposed model for Mg concentration decrease with PCA. (b) Most of the MgO is diffused into the IFL and formed Mg silicate under low a temperature environment. (c) Under a high temperature environment, Mg which does not react with SiO_2 is diffused out from HfO_2.