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Improvement in the asymmetric Vfb shift of poly-Si/HfSiON/Si by inserting oxygen diffusion barrier layers into the interfaces

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1. Introduction

Hf-based materials are good candidates of high-k gate dielectrics for low power consumption CMOS-LSIs. However, the asymmetric flatband voltage (Vfb) shift has been widely reported at poly-Si/Hf-based systems [1-5]. This phenomenon results in high Vth of FETs and makes the applicability of these gate insulators to commercial LSIs difficult. In our previous study, we demonstrated that the thick SiO_2 insertion into poly-Si/HfSiON interface improves the anomalous Vfb shift, although the value of Vfb recovery is as small as 0.15 V [6].

In this study, we discuss the design of the interfacial barrier layer for improving the asymmetric Vfb shift at poly-Si/Hf-based dielectrics/Si systems. We find that the Vfb recovery is critically dependent on the preparation process of the barrier layer. In addition, by separating HfSiO spatially from both poly-Si and Si-substrate with rather thick SiO_2, the ideal Vfb values for n^+ and p^+poly-Si capacitors are obtained for the first time. Oxygen out-diffusion from Hf-based materials to poly-Si, which is closely correlated with the shift, is experimentally confirmed. We also practiced the SiON barrier layer, which enables us to suppress the oxygen diffusion and to relax the EOT constraint concurrently.

2. Experimental

HfSiO(N) films were fabricated on HF-cleaned p-Si (100) wafers by MOCVD or sputtering process. Si or SiO_2 cap layers were deposited onto the HfSiO(N) by sputtering at room temperature. In the case of the Si-capped specimen, rapid thermal oxidation (RTO) of Si-cap was performed at 1000°C to form SiO_2-cap. Poly-Si (p^+, n^+) gated MIS capacitors were fabricated using a conventional process with activation anneal in N_2 at 850°C for 30min or at 1000°C for 30sec. CV characteristics were measured at a frequency of 1MHz. To evaluate the asymmetric Vfb shift, we define ΔVfb (p^+, n^+) as Vfb difference between p^+ and n^+ poly-Si devices on p-Si substrate. We prepare ^{18}O-HfO_2 thin film, formed by oxygen isotope ^{18}O as a component of matrix oxide, in order to investigate oxygen out-diffusion from HfO_2 to poly-Si electrode.

3. Results and Discussion

Figure 1 shows the effect of the preparation process of SiO_2 cap layer on ΔVfb (p^+, n^+) of the poly-Si/HfSiO. As shown in Fig. 1(a), ΔVfb (p^+, n^+) value is ~ 0.4 V in case of the PVD-Si based SiO_2 cap layer as we already reported [6]. In contrast, we can improve ΔVfb (p^+, n^+) as large as 0.7 V, by sputtered SiO_2 (Fig. 1(b) and Fig. 2). These results clearly demonstrate that the improvement in the asymmetric Vfb shift critically depends on the deposition process of the buffer layer even if the buffer material is the same. Furthermore, we inserted thick SiO_2 layers between HfSiO and Si substrate. As shown in Fig. 3(a), the top and bottom SiO_2 layer thickness were 4.2nm and 3.6nm, respectively. Figure 3(b) reveals that Vfb values were completely improved. Figure 4 shows Tphys-I.L. dependence of Vfb values for poly-Si/SiO_2/HfSiO/SiO_2/p-Si capacitors. It was shown that the asymmetric Vfb shift at poly-Si/HfSiO/Si was gradually improved with increasing Tphys-I.L. Figure 5 shows the ΔVfb (p^+, n^+) dependence on the thickness of top SiO_2 layer in poly-Si/SiO_2/HfSiON/SiO_2/p-Si capacitors, changing the bottom SiO_2 thickness as a parameter. We found that bottom SiO_2 layer is essential for the complete improvement in the shift.

It is proposed that oxygen vacancies (Vo) in HfO_2 cause the shift [7,8]. This model indicates that the extraction of O atom from HfO_2 is the initial stage of Vo formation. On the other hand, the complete suppression of the shift in our SiO_2-sandwiched HfSiO structure (Fig.3) also suggests that blocking oxygen diffusion from HfSiO is a key factor. However, there is no direct evidence of oxygen movement between poly-Si and Hf-based dielectric. Figure 6 shows (a) ^{18}O profiles and (b) ^{16}O profiles in Si/^{18}O-HfO_2 structures after the annealing at various thermal budgets measured by Secondary Ion Mass Spectrometry (SIMS). ^{18}O out-diffusion from ^{18}O-HfO_2 to Si becomes significant at higher thermal budget (Fig. 6(a)). In contrast, ^{16}O in the Si layer decreased at the interface after the 800°C annealing (Fig. 6(b)), meaning the ^{16}O atoms moves to ^{18}O-HfO_2 during the annealing. As shown in Fig. 7, net amount of out-diffused oxygen from ^{18}O-HfO_2 increases with increasing the annealing temperature. In addition, the oxygen out-diffusion phenomenon is more severe in the Si/HfO_2 than that in Si/SiO_2 (Fig. 7). Based on these results, we conclude that Vo formation likely occurs in the Si/HfO_2 system especially under high temperature annealing.

It is apparent that thick SiO_2 insertion into the interfaces (Fig. 3) is far from realistic because of its severe EOT increase. In order to lessen the EOT penalty with reasonable Vfb recovery, a thin SiON buffer layer with higher k than that of SiO_2 was practiced (Fig. 8). As shown in Fig. 9, Vfb for the p^+poly-Si device moves 200mV toward ideal Vfb by inserting the SiON layer. We think that such partial improvement in Vfb for p^+poly-Si device makes the application of poly-Si/HfSiON-MIS stack to near future LSTP CMOS-LSIs more realistic. Oxygen depth profiling in the poly-Si/HfSiON/Si structures with and without the top SiON layer clearly shows that oxygen out-diffusion into poly-Si was significantly suppressed by the SiON insertion (Fig. 10).

4. Conclusion

We found that the Vfb shift improvement in the poly-Si/SiO_2/HfSiO structure is dramatically dependent on the preparation method of the SiO_2 layer. Ideal Vfb values for poly-Si/HfSiO/Si-sub. MIS capacitors were successfully demonstrated by separating HfSiO from both poly-Si and Si-sub. We propose that the inhibition of oxygen movement from Hf-based materials to poly-Si is an effective approach for making the application of Hf-based high-k gate dielectrics to low-power consumption CMOS logic more realistic in the near future.

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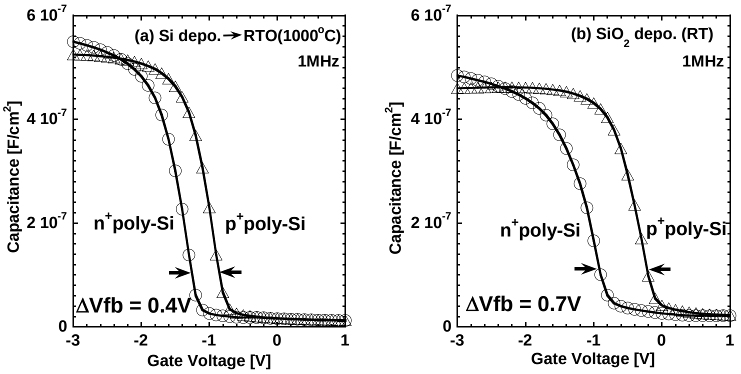

Fig.1 C-V characteristics of poly-Si/SiO_2/HfSiO/I.L./p-Si capacitors. SiO_2 cap layer was formed by (a) RTO (1000°C) and (b) sputter SiO_2 (RT).

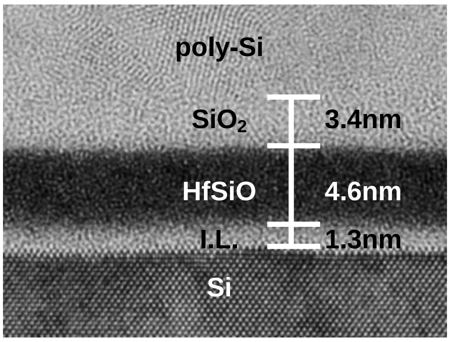

Fig.2 Cross-sectional TEM image of poly-Si/SiO_2/HfSiO/I.L./p-Si stack that C-V characteristics are shown in Fig. 1(b).

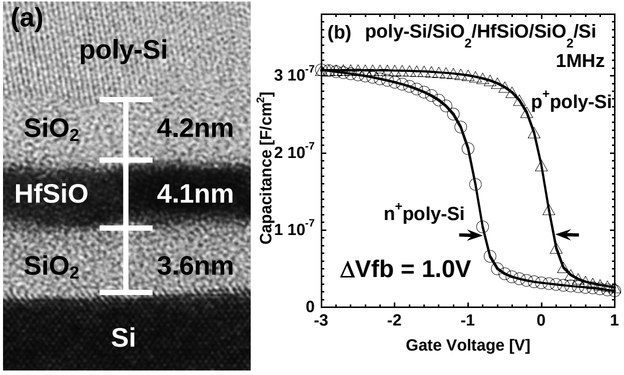

Fig.3 (a) Cross-sectional TEM and (b) C-V characteristics of poly-Si/SiO_2/HfSiO/SiO_2/p-Si capacitors. The asymmetric Vfb shift was completely improved.

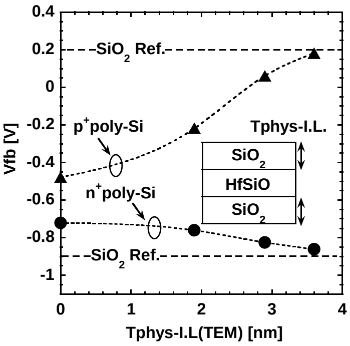

Fig.4 Tphys-I.L. dependence of Vfb values for poly-Si/SiO_2/HfSiO/SiO_2/p-Si capacitors.

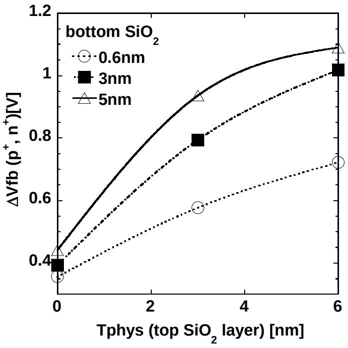

Fig.5 Dependence of ΔVfb (p^+, n^+) on the Tphys of top SiO_2 layer in poly-Si/SiO_2/HfSiON/SiO_2/p-Si capacitors.

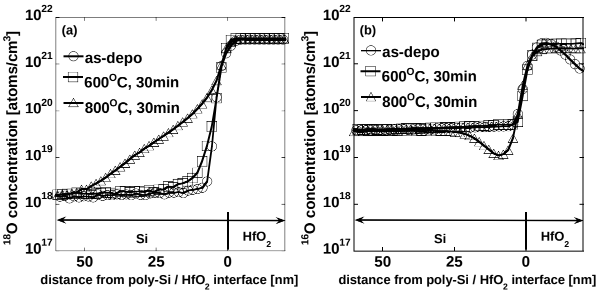

Fig.6 (a) ^{18}O profiles and (b) ^{16}O profiles in Si electrode /^{18}O-HfO_2/Si substrate structures after the annealing at various thermal budgets.

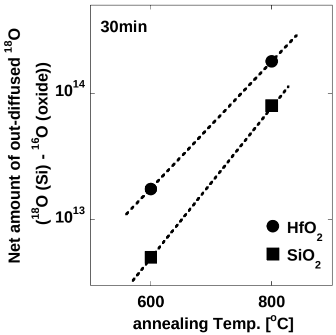

Fig.7 Comparison of the amounts of oxygen out-diffusion from HfO_2 and SiO_2 by annealing.

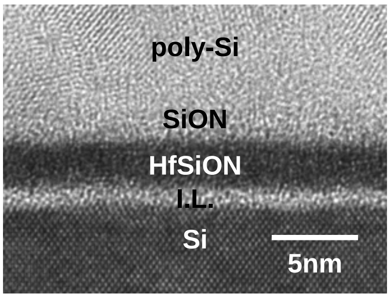

Fig.8 Cross-sectional TEM image of poly-Si/SiON/HfSiON/I.L./Si stack.

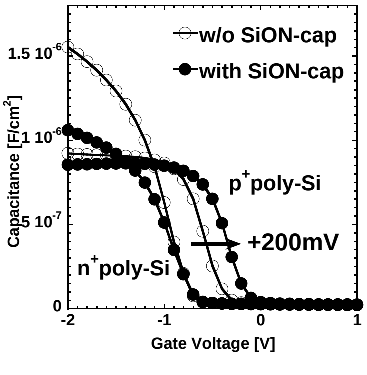

Fig.9 Improved Vfb shift by inserting SiON cap layer into poly-Si/HfSiON interface.

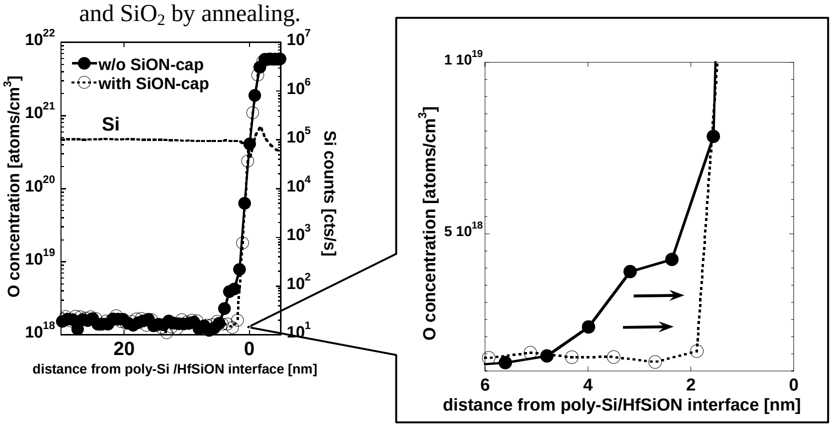

Fig.10 Oxygen Profiles in poly-Si after activation anneal (850°C, 30min) with or without SiON-cap layer on HfSiON.