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Precise Extraction of Metal Gate Work Function from Bevel Structures

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1. Introduction

Up to the present, the metal gate work function has been presented by many researches. However, these values have not been shown as a consistent value because the work function generally varies depending on process conditions, device materials or device structures associated with Fermi level pinning effect. Furthermore, many reports have extracted the work functions from a small number of EOT-V_{FB} plots, which has a risk of leading to their wrong extractions. In this paper, we present precise extractions of metal work function in gate-HfO_2-SiO_2 systems with bevel oxide structures and also provide a guide to understand the work function variations on these MOS systems.

2. Device Fabrication

Fig. 1 shows the device process flow for this study. MOS capacitors were fabricated on 200 mm p-type silicon substrates. All the substrates had 0.7 nm chemical oxides on the surfaces after surface cleaning. 40 nm high temperature oxide (HTO) films were deposited at 730°C. The HTO films were etched down to a thickness range of 0-15 nm with bevel structures. The bevel oxide structure offers a series of oxide thicknesses on the same wafer, hence the reliable and precise extraction of work function from numerous EOT-V_{FB} plots. 3 nm ALD-HfO_2 films were deposited after/prior to the HTO films. Post deposition anneal was carried out at 600 °C for 15 minutes in N_2 ambient. 10 nm CVD-TiN was used as a metal gate material and deposited at 680 °C on the stacked dielectrics. No post metallization anneal was performed except for a final forming gas anneal at 425 °C for 30 minutes. Poly-Si gated capacitors stacked with the same dielectrics were also fabricated as controls. Capacitors with 5 nm and 10 nm uniform HTO films on/under 3 nm HfO_2 were fabricated instead of the bevel HTO to corroborate the results of the capacitors with bevel oxide. NCSU CVC program [1] was used to extract EOT and V_{FB} values. These results were also verified by our extraction program.

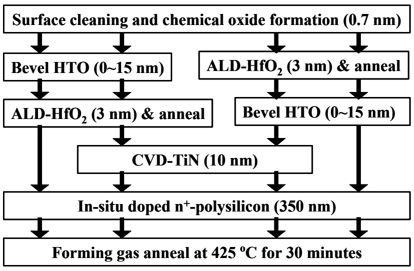

Figure 1: Device fabrication flow

3. Device Characteristics and Discussion

Fig. 2 shows the EOT-V_{FB} plots of TiN/HfO_2/SiO_2/Si stacks with bevel structures. The plots of the capacitors with 5 nm and 10 nm HTO are also given for comparison. This figure clearly depicts a linear relation between EOT and V_{FB} down to 2 nm, from which the work function of 4.83 eV is extrapolated. The plots of stacks with fixed HTO thickness are on the extrapolated line without any inconsistency, so validating the extraction of the work function from the bevel oxide structure. A rollover in V_{FB} is observed when the EOT is less than 2 nm. Two possibilities are conceivable: one is that the HTO was totally etched off; as a result, the HfO_2 formed on the HTO came on the Si substrate through 0.7 nm chemical oxide by intermixing and created an extra interface charge. The other possibility is caused by nitrogen diffusion onto the Si surface through HfO_2 during TiN formation [2]. An abrupt increase in the equivalent oxide charge density for EOT values less than 2 nm shown in the inset of Fig. 2 supports these explanations.

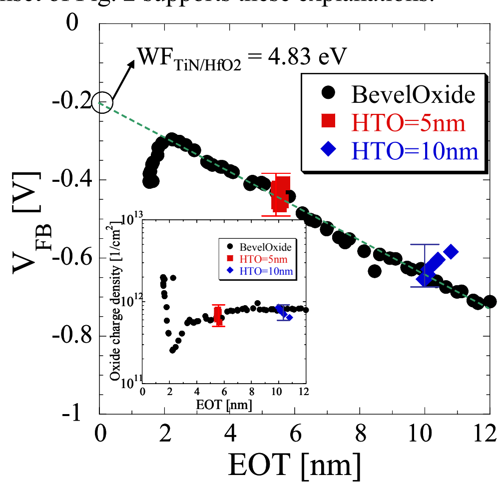

Figure 2: EOT-V_{FB} plot of TiN/HfO_2/SiO_2/Si stacks with bevel oxide. The capacitors with fixed SiO_2 thickness of 5 nm and 10 nm instead of the bevel oxide are also plotted. The inset exhibits EOT-oxide charge density plot.

Fig. 3 shows the EOT-V_{FB} plots of TiN/SiO_2/HfO_2/Si stacks with bevel structures. In contrast to TiN/HfO_2 case, the plots do not show a proportional relation throughout the EOT range. In a range of EOT between 7-12 nm, the work function is found to be 4.36 eV and from a range between 5-7 nm, V_{FB} changes abruptly resulting in the plural extraction of work function. In a range between 2.5-5 nm, the work function is found to be 4.54 eV. Moreover, in a range less than 2.5 nm, V_{FB} again changes abruptly and finally reaches almost the same value as that of TiN/HfO_2 case (cf. Fig. 2). One can find, as a result, three different characteristics due to two abrupt changes in V_{FB}. Based on these results, we speculate that there exist three interfaces in this structure: the first is the TiN/SiO_2 interface in a large EOT range (EOT=7-12 nm), hence no Hf atom is present at the interface; the second is the TiN/Hf-silicate interface (EOT=2.5-5 nm) where both Hf and Si atoms are present at the interface by intermixing; the third is the TiN/HfO_2 interface where no Si atom is present due to complete HTO etching. These considerations suggest that the TiN work function highly depends on the dielectric component at the interface, especially a presence of Si atoms. The equivalent oxide charge density shown in the inset of Fig. 3 depicts no abrupt change indicating a stable HfO_2/Si interface and also corroborating the explanation of the rollover in Fig. 2.

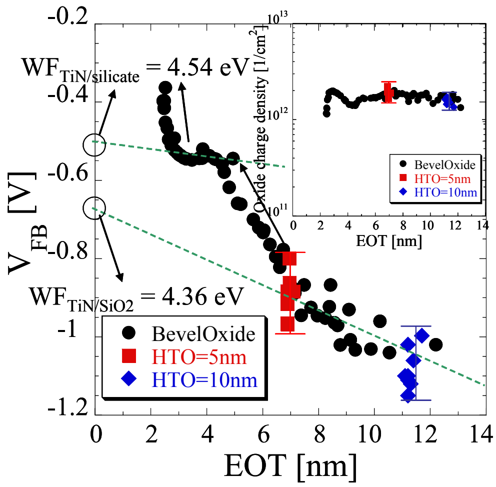

Figure 3: EOT-V_{FB} plot of $TiN/SiO_2/HfO_2/Si$ stacks with bevel oxide. The capacitors with fixed SiO_2 thickness of 5 nm and 10 nm instead of the bevel oxide are also plotted. The inset exhibits EOT-oxide charge density plot.

Fig. 4 shows EOT-V_{FB} plots of n^+-poly-$Si/HfO_2/SiO_2/Si$ stacks with bevel oxides. The extracted work function is found to be 4.28 eV which is a higher value than that of n^+-poly-$Si/SiO_2/HfO_2/Si$ (as low as 4.03 eV, not shown). A rollover seen in Fig. 4 could also be explained by the HfO_2 film on the Si substrate through the chemical oxide by intermixing, which leads to an increase in the oxide charge density as shown in the inset of Fig. 4.

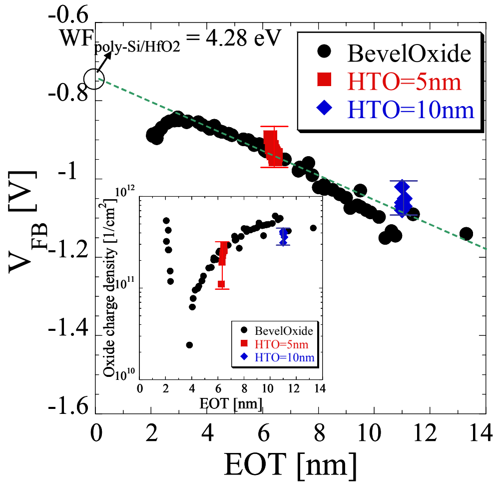

Figure 4: EOT-V_{FB} plot of n^+-poly-$Si/HfO_2/SiO_2/Si$ stacks with bevel oxide. The capacitors with fixed SiO_2 thickness of 5 nm and 10 nm instead of the bevel oxide are also plotted. The inset shows EOT-oxide charge density plot.

Fig. 5 summarizes the work functions extracted from this study. The work function of n^+-poly-Si/HfO_2 structure shifting to about 4.3 eV is due to Hf-Si bonds and is also consistent with other experimental and modeling studies [3, 4]. It should be noted that the $TiN/SiO_2/HfO_2$ stack shows two work functions of 4.36 eV and 4.54 eV depending on the SiO_2 thickness, while $TiN/HfO_2/SiO_2$ stack shows the sole value of 4.83 eV. Here, we argue four facts: the first is that the Fermi level pinning effect occurs on both TiN and poly-Si gate depending on the metal/dielectric interfaces [5]; the second is that the Fermi level pinning effect on the n^+-poly-Si is rather weak compared to that on TiN [4]; the third is that the work functions of both $TiN/SiO_2/HfO_2$ and n^+-poly-$Si/HfO_2/SiO_2$ stacks converge to a value of about 4.3 eV; the fourth, based on the work function dependence on SiO_2 thickness (Fig. 3), is that the TiN work function is likely to depend on the amount of Si atoms at TiN/SiO_2 interface [6]. However, assuming extrinsic states between TiN and SiO_2, Ti-Si bonds should produce a negative dipole charge at the dielectric side, resulting in the work function pinned at the more positively biased side. Thus, Fermi pinning with the bonding theory explained in [5] is inconsistent with our result. The cause for this inconsistency is now under investigation.

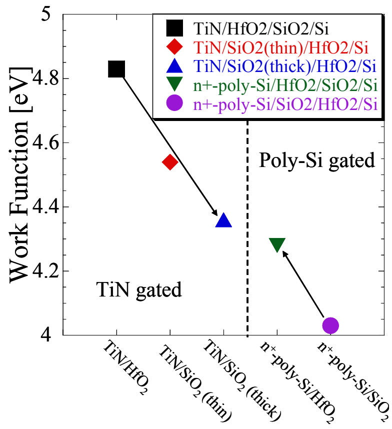

Figure 5: Transition of work function with various metal/dielectric interfaces.

4. Conclusions

The work functions of CVD-TiN and n^+-poly-Si on different gate dielectrics were investigated with the bevel oxide structures. The reliable work function extraction was demonstrated from a wide range of continuous EOT values enabled by the bevel oxide structures. The work functions of both TiN and n^+-poly-Si were found to depend on the underlying dielectrics, especially TiN gate showed a larger shift than the n^+-poly-Si gate. TiN on HfO_2/SiO_2 exhibited a work function value of 4.83 eV, while TiN on SiO_2/HfO_2 showed two work function values of 4.36 eV and 4.54 eV depending on the SiO_2 thickness. The poly-Si on HfO_2 showed a work function value of 4.28 eV which is consistent with several reports. Both TiN/SiO_2 and poly-Si/HfO_2 stacks showed the work function shifts toward about 4.3 eV due to the Fermi level pinning effect most likely caused by Ti-Si and Si-Hf bonds respectively.

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