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Material Selection for the Metal Gate/High-k Transistors

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1. Abstract

The material dependence of the gate leakage current and transistor performance are systematically investigated using 7 kinds of metals for the gate electrode of HfSiON MISFETs. For n^+ poly-Si and metals, the Vfb of HfSiON MISFETs are almost the same as those of SiON MISFETs. Only p^+ poly shows a large Vfb shift. The leakage current of metal nitride-gated MISFETs is almost propotional to the density of oxigen vacancies in the high-k insulator. The leakage current of the metal nitride gated MISFETs meets the target of LOP of 65nm node. It was found that the low leakage current and small work function suitable for NMISFET could obtain at the same time by using ZrN gate electrode.

2. Introduction

The large Vth shift of n^+/p^+ poly-Si gate is one of the main concerns for the Hf-based high-k MISFETs. The difficulty of Vth control has accelerated the researches of the metal gate high-k transistors. The effective work function of the metals on HfO_2 based high-k insulators was extensively studied[1][2]. On the other hand, the reactivity of the metal/high-k interface has not been forcused on in the discussion of the transistor characteristics.

In Fig.1, the work functions of several metals are plotted as a function of the standard heat of formation of metal oxides. Considering only the work function leads to the speculation that metals near the dashed lines are suitable for N and PMISFET, respectively. However, there exists a trade-off relationship between the work function and the reactivity. The larger absolute value of the heat of formation (the left side) corresponds to high reactivity of the metals with the oxide such as high-k materials. Fig.1 is indicative that the metals suitable for NMIS are highly reactive with the oxide. Therefore, the less-reactive gate material for NMISFET is strongly needed for realization of the high-k metal gate MISFETs. In this study, the influence of the reactivity on the MISFET's characteristics and the effective work function are systematically investigated for the material selection.

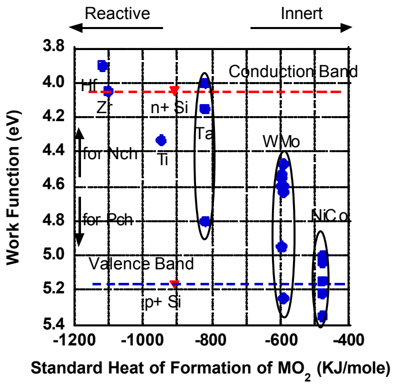

Fig.1 The relationship between the heat of formation of metal oxides and the work function of the metal

3. Experiments

The MISFETs were fabricated by the replacement gate process as shown in Fig.2 [3]. The gate insulator and the gate electrode were formed after the source/drain activation. Because of the low thermal budget after the gate formation, even reactive metals can be used as the gate electrodes. For the direct comparison of metals and poly-Si, HfSiON is selected as a high-k film because it is durable for the activation of the doped poly-Si. $HfSiO_x$ films with the thickness 3nm were deposited by MOCVD followed by O_3 treatment and NH_3 nitridation [4]. SiON films were used as references. Ti, TiN, Ta, TaN, Mo, MoN, ZrN and n^+/p^+ poly-Si were used as the gate materials. Ti and TiN were deposited by $TiCl_4$-based CVD at 450C and 650C respectively. Ta and Mo were deposited by sputtering. TaN, MoN and ZrN were deposited by reactive sputtering. The poly-Si films were doped with P^+ and B^+ implantation followed by RTA at 1000C for 3sec. FG annealing at 400C for 30min was carried out after wiring formation. EOT and Vfb are calculated by the NCSU CVC program [5].

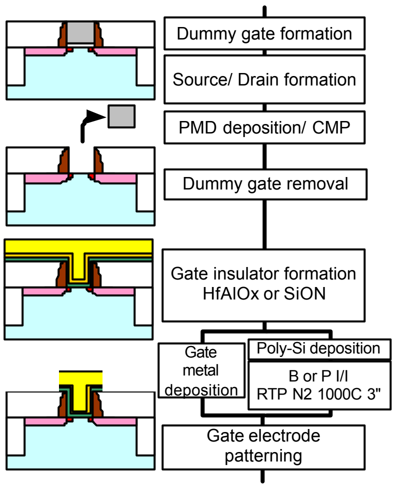

Fig.2 The schematic flow of the replacement gate process

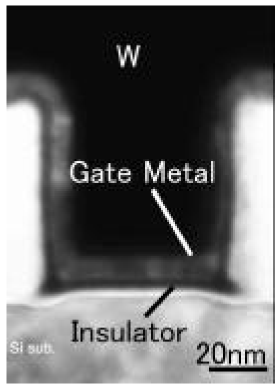

Fig. 3 A cross-sectional TEM image of the metal/ high-k gate MISFET

4.Results and Discussion

4-1. Influence of Reactivity of the Metals

Fig.3 shows a cross-sectional TEM image of the replacement metal gate MISFET.

The effective work function on SiON and the Metal/ Nitrogen ratio measured by RBS (Rutherford Backscattering Spectroscopy) is summarized in Table I. From the viewpoint of effective workfunction, ZrN and Ta are suitable for NMISFET and TiN is suitable for PMISFET.

Fig.4 shows the relationship between the Vfb values of the HfSiON MISFETs and the SiON MISFETs. The Vfb value of the Ti gate MISFET could not be calculated because of the large leakage current. The Vfb's in SiON and HfSiON MISFETs show an almost linear relationship

Material	Φm(eV)	N/Metal
n+ poly	4.05	
ZrN	4.25	1.00
Ta	4.34	-
Mo	4.51	-
TaN	4.54	1.75
MoN	4.56	1.00
TiN	4.77	1.04
p+poly	5.07	

Table I Summary of Effective Work Function and the atmic ratio of Nitorogen/Metal

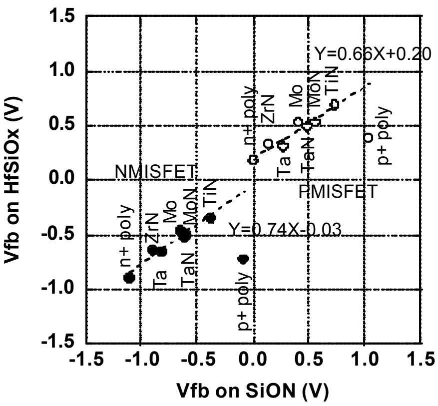

Fig.4 The relationship between the Vfb's of SiON and HfSiON MISFETs. Only p+ poly on HfSiON shows large shift

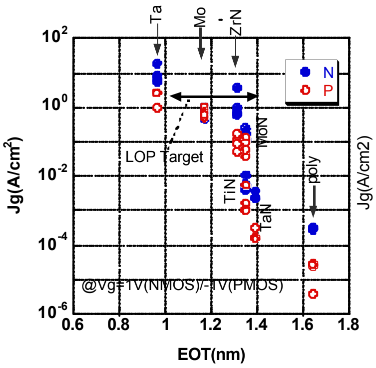

Fig.5 Relationship between EOT and Jg at Vg=1V(N)/-1V(P). EOT thinning is observed in pure metals.

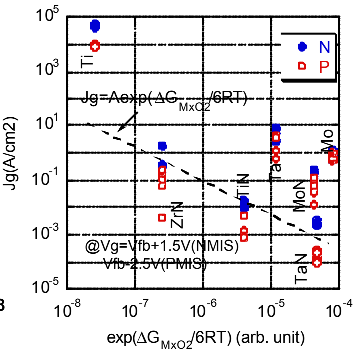

Fig.6 The correlation between $\exp(\Delta G_{MxO2}/6RT)$ and Jg . ΔG_{MxO2} is the heat of formation of the metal oxide (MxO_2)

except for that of p^+ poly-Si gate. Dashed lines were the least-squares fits excluding p^+ poly-Si. The changes in Vfb of the metals and n^+ poly-Si on HfSiON gate insulator are smaller than for SiON. Since similar results were already reported for HfO_2[6][1], this result indicates that the MIGS (Metal Induced Gap State) theory is applicable to the system consisting of a combination of a wide variety of metallic materials and HfSiON. The large shift of p^+ poly-Si is well explained by the oxygen vacancy model that considers both the work function and the reactivity of the gate materials [7].

Fig.5 shows the relationship between EOT and gate leakage current at Vg=+-1V in inversion in HfSiON MISFETs. EOT thinning is observed in the highly reactive metals such as Mo, Ta and Ti. Enhancement of the leakage current observed in these metals is caused by EOT thinning. Formation of the metal-nitrogen bond is thought to be effective for the suppression of the reaction between metal and high-k insulator.

In the case of metal nitrides, EOT is 0.25-0.3nm thinner than poly-Si. This result is in good agreement with the reported value [8]. Metal nitride gates meet the target of leakage current of 65nm LOP [9].

It was reported that the density of the oxygen vacancy in HfO_2 is proportional to $\exp(-\Delta G_{MxO2}/6RT)$, where ΔG_{MO2} is the heat of formation of metal dioxides (M_xO_2) [10]. Fig.6 demonstrates the correlation between $\exp(\Delta G_{MxO2}/6RT)$ and Jg. In the case of nitride, Jg is almost proportional to $\exp(\Delta G_{MxO2}/6RT)$. This result suggests that the leakage current is caused by the oxygen vacancy even in HfSiON in the case of metal nitride. Pure-metals show larger leakage currents than metal nitrides, which is considered to be the result of the EOT thinning.

4-2. MISFET Characteristics

Based on the discussion above, we have selected ZrN and TiN as N and P metals, respectively. Fig.7 shows the Vth. roll-off characteristics. Fig.8 shows the subthreshold characteristics of the ZrN NMISFET with the gate length of 90nm and the TiN PMISFET with the gate length of 70nm. The difference between Vth of n^+ poly and ZrN NMISFET at Lg=10000nm is 0.17V, which is tunable by channel engineering. In TiN PMISFET, the Vth is 0.35V smaller than for p^+ poly.

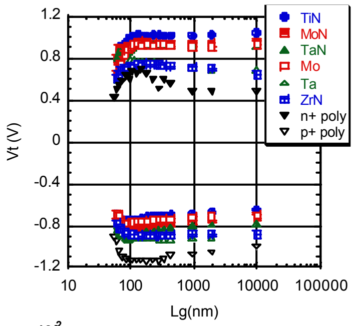

Fig.7 Vth roll-off of the metal gate/HfSiON MISFETs.

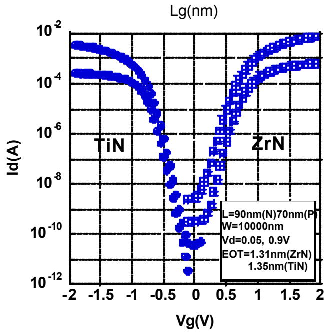

Fig.8 The subthreshold characteristics of the L=90nm ZrN NMISFET and L=70nm TiN PMISFET. EOT=1.31nm (ZrN)/ 1.35 (TiN)

5. Conclusion

Vfb's of HfSiON metal gates are similar to those of SiON. In the case of pure metals, EOT thinning was observed due to high reactivity between metal and high-k insulator. The acceptable Vt's are obtained in ZrN NMISFET and TiN PMISFET. The leakage currents of metal nitride gates meet the target of 65nm node LOP. ZrN and TiN are good candidates for HfSiON metal gate MISFETs from the view points of both work function and reactivity.

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