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⁺ polysilicon shows a large Vfb shift. The leakage current of metal nitride-gated MISFETs is almost proportional to the density of oxygen 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 metal on HfO₂ has not been studied extensively [1][2]. On the other hand, the reactivity of the metal/high-k interface has not been investigated 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 metal/high-k interface has not been systematically investigated for the metal selection.

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. HfSiO₂ films with the thickness 3nm were deposited by MOCVD followed by O₂ treatment and NH₃ 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 TiCl₄ 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].

4. Results and Discussion

4-1. Influence of Reactivity of the Metals
Fig.3 shows a cross-sectional TEM image of the replacement gate metal 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 HfSiO₂ and HfSiON MISFETs show an almost linear relationship.
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 HfO2, it is expected that the MISFETs with HfSiON as gate insulator are more resistant to EOT thinning than metal nitrides, which is considered to be the result of the EOT thinning.

In the case of nitride, Jg is almost proportional to exp(ΔG/6RT) and Jg is the heat of formation of the metal oxide (MxO2). This result suggests that the leakage current is caused by the oxygen vacancy even in HfSiON. In the case of pure metals, EOT thinning was observed due to high reactivity between metal and high-k insulator. The acceptable Vth’s are observed 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 viewpoint of both work function and the reactivity of the metal materials and HfSiON. In the case of pure metals, EOT thinning was observed due to high reactivity between metal and high-k insulator. The acceptable Vth’s are observed 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 viewpoint of both work function and reactivity.

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 Vth’s are observed 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 viewpoint of both work function and reactivity.

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References

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