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Investigation of the Interface Stability of the Metal/HfO_2/AlN/InGaAs MOS Devices

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Abstract

The stability of (Mo, Ni, Pd)/HfO_2 interfaces was studied in this paper. The oxidations at the Mo/HfO_2 and the Ni/HfO_2 interfaces were found to have no effect on the quality of HfO_2 film; however, the formation of the interfacial layer PdO_x at the Pd/HfO_2 interface considerably increased the oxygen vacancies in the HfO_2 film. Low dissociation energy for the Pd-O bond was attributed to oxygen segregation, leading to the increase of mobile O^{2-} and OH^- ion densities during annealing. The results provide the guidance for choosing the proper metal electrode for the InGaAs based MOSFET.

1. Introduction

Hafnium-based oxides are recently considered as promising candidates as the high-k dielectric for III-V channel devices. The reactions between the metal electrode and the oxide layer may lead to the degeneration of the oxide layer. Yoshida et al.[1] recently reported that the reactions between the high-k material and InGaAs were due to the interaction at the metal/oxide interface. To suppress this interfacial interaction, the passivation of HfO_2/InGaAs interface using AlN layer was reported.[2] Therefore, the mechanism suggested by Yoshida et al. should be complemented when a non-oxide layer is used to passivate the HfO_2/InGaAs interface. In this study, the oxygen segregation at the (Mo, Ni, Pd)/HfO_2 interfaces of the HfO_2/AlN/InGaAs MOSCAP is investigated. Mo was chosen due to its low work function applicable for NMOS InGaAs devices, while Ni and Pd were chosen because of their high work function suitable for PMOS InGaAs devices.

2. Experimental

The MOSCAP was fabricated on the 100-nm epitaxial $In_{0.53}Ga_{0.47}As$ layer ($5 \times 10^{17}/cm^3$ Si-doped n-type wafer). First, the wafer went through an HCl: H_2O (3.8%) solution treatment for 2 minutes before it was loaded into the ALD chamber. Then, 0.8-nm AlN layer and 50 cycles HfO_2 were deposited on the InGaAs layer. After that, the samples were annealed in forming gas (FG) at 450 ^oC for 5 minutes using rapid thermal annealing (RTA). Three types of metal including Mo, Ni, and Pd were studied as the gate metals on the HfO_2 layer. The gate metals were deposited through E-gun evaporation with the based pressure about 3×10^{-7} torrs. The AuGeNiAu was deposited on the backside of the wafer to form the ohmic contact. Finally, the MOSCAPs were annealed in three different ambiances including FG, nitrogen (N) and oxygen (O) at 350 ^oC for 30s using RTA for comparison.

Table I The area percentage (%) of O^I, O^{II}, and O^{III} peaks of the clean HfO_2 surface, Mo/HfO_2 interface and Pd/HfO_2 interface.

$O^i/(O^I+O^{II}+O^{III})$	Clean HfO_2	Mo/HfO_2	Pd/HfO_2
O^I	85.4	79.8	33.0
O^{II}	8.5	9.5	41.7
O^{III}	6.1	10.7	25.3

3. Result and discussion

Figure 1(a) shows the capacitance-voltage (C-V) hysteresis (ΔV_{FB}) of the (Mo, Ni, Pd)/HfO_2/AlN/InGaAs MOSCAPs. The fact that the ΔV_{FB} of the Pd MOSCAP is very large (~ 1V), while the ΔV_{FB} of the Mo MOSCAP is very small (~ 0.11 V) indicates that a large number of bulk oxide traps was created after Pd was deposited on HfO_2 and annealed in FG. Based on the thermodynamics, the ΔC_{acc} of the Mo MOSCAP should be larger than the ΔC_{acc} of the Pd MOSCAP because the Mo-O reaction (oxidation formation enthalpy ΔH ~ – 178 kCal/mol) is more exothermal than the Pd-O reaction (ΔH – 49.9 kCal/mol). However, the opposite results were observed in Fig. 1(b), indicating that the oxidation at the Pd/HfO_2 interface is not the only reason for the oxide degeneration for the Pd/HfO_2/AlN/InGaAs MOSCAP. Instead, an unstable interfacial layer (IL) PdO_x at the Pd/HfO_2 interface should be attributed to the oxygen segregation at the Pd/HfO_2 gate stack. Fig. 1(c) and 1(d) show the leakage currents and the D_{it}, respectively, for the three MOSCAPs. The leakage currents of the three MOSCAPs at V_{FB} + 1 (V) were in the range of 2×10^{-8} A/cm^2 ~ 6×10^{-8} A/cm^2, indicating that the HfO_2/InGaAs interface was totally passivated by AlN IL layer. The low D_{it} values (~ 4×10^{12} $cm^{-2}eV^{-1}$ determined from Terman method) of

the Ni MOSCAP and the Mo MOSCAP, shown in Fig. 1(d), are in agreement with the previous reports.[2] Note that Terman method gives both slow and fast traps and provides a reliable value for Dit at midgap. Fig. 1 also shows that the PMA process has little effect on the electrical characteristics of the Ni MOSCAP; thus, Ni is a more suitable gate metal for the InGaAs based p-MOSFET.[2].

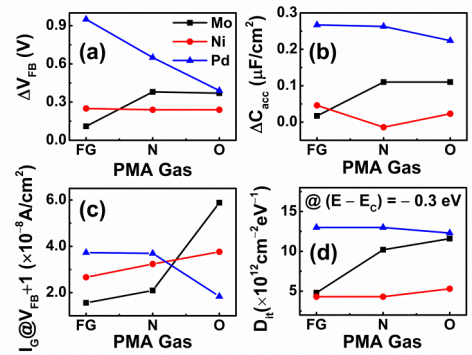

Fig. 1 The electrical characteristics of (Mo, Ni, Pd)/HfO_2/AlN/InGaAs MOSCAPs after PMA in FG, N, and O ambient gases at 350 °C for 30s, (a) the hysteresis at V_{FB} of the 1 MHz C-V curves after PMA, (b) the C_{acc} variation of the MOSCAPs after PMA measured at +2 V and 1 MHz; the C_{acc} variation equals C_{acc} before PMA minus C_{acc} after PMA. (c) The leakage currents of the MOSCAPs at V_{FB} + 1 (V) after PMA and (d) the D_{it} at E – E_C = – 0.3 eV from the conduction band edge of the MOSCAPs after PMA.

The dissociation energies (D_S) of the metal-oxygen bonds for the metals used in this study are Mo-O bond (119.9 kCal/mol), Ni-O bond (87.42 kCal/mol), and Pd-O bond (53.87 kCal/mol). It can be seen that PdO_x is easier to decompose during the PMA process compared to other oxides in this study following the equation:

$$PdO_x \rightarrow Pd^{2+} + xO^{2-}. \quad (1)$$

The O^{2-} ions can easily diffuse into the Pd layer, leading to the formation of a thick PdO_x IL at the Pd/HfO_2 interface as shown in Fig. 2(a). This IL was not found at the Ni/HfO_2 interface as shown in Fig. 2(b). Fig. 2(c) shows the Energy-dispersive X-ray spectroscopy (EDS) spot profile of the PdO_x IL. An oxygen percent of ~ 24 % was found in the PdO_x layer, indicating a significant internal diffusion of the O^{2-} ions from the HfO_2 layer into the Pd layer. Fig. 2(d) and (e) show the scanning electron microscope (SEM) images of the Pd MOSCAP and the Ni MOSCAP, respectively, after RTA in FG at 400 °C for 5 minutes. Some bubbles occurred at the surface of the Pd MOSCAP, indicating that the Pd MOSCAP was destroyed due to the diffusion of O^{2-} ions from the HfO_2 layer into the Pd layer.

The high percentage of XPS O^I peak as shown in Fig. 3 and Table 1 for clean HfO_2 surface refers the high quality of ALD HfO_2 film. The O 1s peak of the Mo/HfO_2 interface is same as the O 1s peak of the clean HfO_2 surface, indicating that the Mo/HfO_2 interface is quite stable due to the large dissociation energy of the Mo-O bond. For the Pd/HfO_2 interface, it was found that the O^I intensity decreased from 85.4 % for the clean HfO_2 surface to 33 % for the Pd/HfO_2 interface as shown in Table 1. The considerable increase of the intensities of the O^{II} and O^{III} peaks at the Pd/HfO_2 interface indicates a significant increase of the oxygen vacancies in HfO_2, due to the diffusion of O^{2-} ions from the HfO_2 layer to the Pd layer.

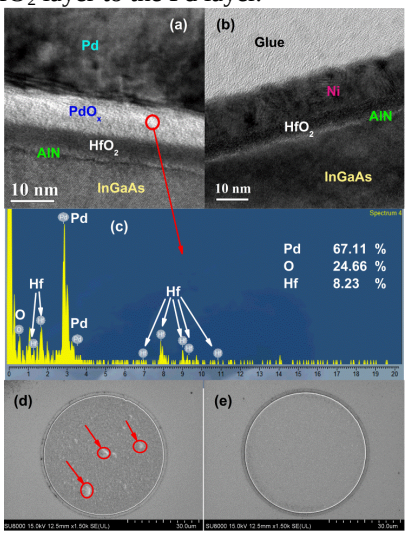

Fig. 2 (a) and (b) Transmission electron microscopy (TEM) cross sections of Pd/HfO_2/AlN/InGaAs and Ni/HfO_2/AlN/InGaAs structures, respectively, (c) the EDS spot profile of the interfacial layer PdO_x at the Pd/HfO_2 interface, (d) and (e) SEM images of the patterns of Pd/HfO_2 and Ni/HfO_2 MOSCAPs, respectively, after RTA in FG at 400 °C for 5 minutes.

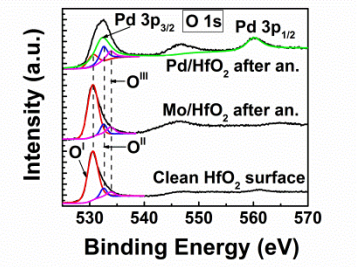

Fig. 3 XPS spectra of O 1s peaks of clean HfO_2 surface, Mo/HfO_2 and Pd/HfO_2 interfaces after PMA in FG at 350 °C for 30s,.

3. Conclusion

The oxidations at the Mo/HfO_2 and the Ni/HfO_2 interfaces were found to have no effect on the quality of the gate stack; however, the formation of the interfacial layer PdO_x at the Pd/HfO_2 interface considerably increased the oxygen vacancies in the HfO_2 film. The unstable PdO_x layer contains the O^{2-} and OH^- ions, which are mobile during annealing.

Acknowledgements

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