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Determining factor of effective work function in metal/bi-layer high-*k* gate stack structure studied by photoemission spectroscopy

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Introduction

Recently, metal/high-dielectric oxide (high-*k*)/Si gate stack structures with LaO_x and AlO_x cap layers have been studied due to excellent controllability of effective work function (EWF) in complementary metal-oxide-semiconductor devices, after high-temperature thermal annealing for dopant activation. The physical origin of change in the EWF is considered to be due to magnitude of microscopic dipoles at the high-*k*/SiO_2 interface, which is readily modulated by diffusion of La or Al atoms from the cap layer. Investigation of the determining factor of EWF only by electrical measurements involves some difficulties, because there are few methods to reveal chemically and electronically resolved depth distribution of metal/high-*k* gate stack structures. We have previously analyzed depth profiles of atomic concentration and contribution of the interface dipoles in TiN/LaO_x/HfSiO/SiO_2 stack structures by angle-resolved core-level photoemission spectroscopy, which is expected to be one of the promising candidate techniques to experimentally elucidate the determining factor of EWF in metal/high-*k* gate stack structures [1]. In this study, we have focused on bi-layer HfO_2/Al_2O_3 high-*k* materials on SiO_2/Si substrates, and investigated the effects of a Si interlayer among the bi-layer high-*k* materials.

Experimental

1.0 nm HfO_2 and 1.0 nm Al_2O_3 dielectric layers were grown on 1.0 nm SiO_2 interface layers on Si substrates. Si layers are inserted at the HfO_2/Al_2O_3 (Sample A) and Al_2O_3/SiO_2 (Sample B) interfaces as interface passivation layers. The EWFs are determined to be 4.93 and 4.96 eV for samples A and B by *C-V* characteristics, respectively. Finally, 15 nm TiN and thick poly-Si for gate electrodes were also deposited. Photoemission measurements were performed at BL-2C of the Photon Factory in the High Energy Accelerator Research Organization (KEK), which is equipped with a high performance photoelectron analyzer (VG-SCIENTA SES2002). Photoelectron emission angles were changed from the surface normal to 75° for enhancement of surface sensitivity.

Results and Discussion

Figure 1 shows depth profiles of atomic concentration in the SiO_2/bi-layer high-*k*/TiN stacked structures for (a) Sample A and (b) Sample B. Inset for each panel indicates the as-grown sample structures. It is found that inserting a Si passivation layer at the HfO_2/Al_2O_3 interface effectively modulates depth profiles of cations such as Al and Hf atoms. The inserted Si layer is completely oxidized during film growth or annealing processes, and outward diffusion of Al atoms into the top HfO_2 layer is suppressed. It is well known that EWF of the Al_2O_3/SiO_2 stack is larger than that of the HfO_2/SiO_2 stack, which is based on the interface dipole model. Since high concentration of Al atoms at the SiO_2 and high-*k* layers should increase EWF by enhancing magnitude of the interface dipole between the SiO_2 and high-*k* layers, the fact that EWF of Sample A is larger than that of Sample B cannot be interpreted only by variation in dipole at the SiO_2/high-*k* interface. Although effect of the interface dipole is suppressed by inserting the Si layer at the HfO_2/Al_2O_3 interface, the Si layer effectively prevents oxygen diffusion from the HfO_2 layer into the TiN metal electrode, resulting in a decrease in the EWF of the TiN metal electrode [2]. Thus, the guideline for high EWF is promotion of TiN metal electrode oxidation at the high-*k*/TiN interface without weakening the magnitude of interface dipole. This can be utilized in fabrication processes of metal/high-*k* gate stack structures.

References

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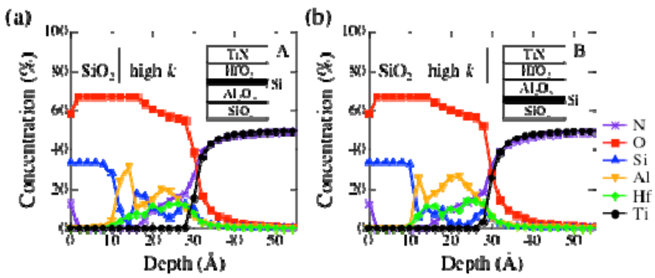

Fig. 1; Depth profiles of atomic concentration in the SiO_2/bi-layer high-*k*/TiN stacked structures. Passivation layers of Si are inserted at the HfO_2/Al_2O_3 (a) and Al_2O_3/SiO_2 (b) interfaces for Sample A and Sample B.