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# Chemical-state resolved depth profile and band discontinuity in TiN/HfSiON gate stack structure with an $AlO_x$ cap layer

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## Introduction

For sub 32 nm complementary metal-oxide-semiconductor (CMOS) devices, metal/high-dielectric metal oxide (high-*k*)/Si gate stacked structures with $LaO_x$ and $AlO_x$ cap layers have been widely studied in order to fine-tune threshold voltages for NMOS and PMOS, respectively. One of the most critical issues to be solved in metal/high-*k* systems is to control the flat-band voltage ($V_{fb}$) after the high-temperature thermal annealing for dopant activation. It is necessary to develop the guidelines for control of the $V_{fb}$ shift in overall stacked structures with a cap layer and to reveal their complicated mechanisms such as Fermi-level pinning and interface-dipole effects. Although the physical origin of the $V_{fb}$ shift has recently been considered to be due to interface dipole at high-*k*/$SiO_2$ interfaces, there are few reports on effects of N bonding state and their changes in depth profiles upon annealing. In this study, we have investigated chemical-state-resolved depth profiles and band discontinuity for TiN/HfSiON gate stack structure with the $AlO_x$ cap layer on a Si substrate using backside angle-resolved photoemission spectroscopy.

## Experimental

The HfSiON dielectric layers were grown by atomic layer deposition (ALD) on $SiO_2$ interface layers. $AlO_x$ capping layers and TiN gate electrodes were also deposited by ALD processes. Rapid thermal annealing was performed. Photoemission measurements were carried out 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). Angle-resolved core-level photoemission spectra from the backside of the gate-stacked structures were measured using synchrotron radiation focused beam of 0.1 x 0.5 $mm^2$. Photoelectron emission angles ($\theta_e$) were changed from the surface normal to 75° for enhancement of surface sensitivity.

## Results and Discussion

Figure 1 shows atomic concentration depth profiles in the $SiO_2$/high-*k*/TiN stacked structures without (a) and with (b) the $AlO_x$ cap layer. Depth profile for each sample shows the anticipated stacked structure except for the position of $AlO_x$ compounds and the distribution of N atoms. In other words, depth profiles related to Al and N atoms are significantly changed upon annealing. Although the $AlO_x$ layer is deposited on the HfSiO layer in the as-grown stage, Al atoms diffuse into the interface between the HfSiON and $SiO_2$ layers during rapid thermal annealing and $AlO_x$ compounds have broad distribution around the HfSiON layer. Core-level intensity ratio of Al 2*p* to Hf 4*f* increases for enhancing surface sensitivity by changing emission angle as shown in the inset of Fig. 1(b), which suggests that $AlO_x$ compounds are highly distributed at the high-*k*/$SiO_2$ interface rather than throughout the high-*k* layer. Such concentration of Al atoms at the high-*k*/$SiO_2$ interface may control the effective work function for PMOS devices. We note that inserting the $AlO_x$ layer also changes distribution of nitrogen atoms in the HfSiON layer. The total amount of nitrogen atoms decreases by $AlO_x$ layers. High nitrogen concentration in the high-*k* layer may be originated from the TiN gate electrode, so the insertion of $AlO_x$ layer prevents excess nitrogen diffusion from the electrode. Thus, it is found that effect of the $AlO_x$ capping layer at the interface of high-*k*/TiN strongly influences depth profile of nitrogen atoms [1].

## References

[1] S. Toyoda *et al*., J. Appl. Phys. **110**, 104107 (2011).

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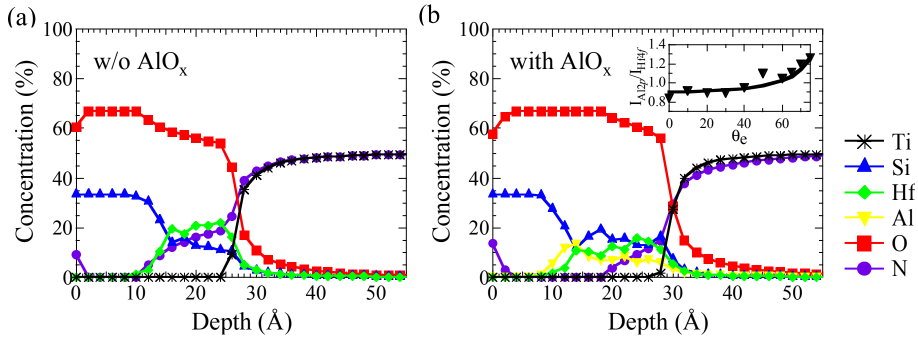


Fig. 1; Depth profiles are analyzed using the angle-resolved core-level intensity with (a) and without (b) $AlO_x$ cap layer. Core-level intensity ratio of Al 2*p* to Hf 4*f* as a function of $\theta_e$ are also shown in the inset of Fig. 1(b).