Chemical-state resolved depth profile and band discontinuity in TiN/HfSiON gate stack structure with an AlO\textsubscript{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\textsubscript{x} and AlO\textsubscript{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 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\textsubscript{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\textsubscript{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\textsubscript{2} interface layers. AlO\textsubscript{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\textsuperscript{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\textsubscript{2}/high-k/TiN stacked structures without (a) and with (b) the AlO\textsubscript{x} cap layer. Depth profile for each sample shows the anticipated stacked structure except for the position of AlO\textsubscript{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\textsubscript{x} layer is deposited on the HfSiO\textsubscript{2} layer in the as-grown stage, Al atoms diffuse into the interface between the HfSiON and SiO\textsubscript{2} layers during rapid thermal annealing and AlO\textsubscript{x} compounds have broad distribution around the HfSiO\textsubscript{2} layer. Core-level intensity ratio of Al 2p to Hf 4f\textsubscript{7/2} increases for enhancing surface sensitivity by changing emission angle as shown in the inset of Fig. 1(b), which suggests that AlO\textsubscript{x} compounds are highly distributed at the high-k/SiO\textsubscript{2} interface rather than throughout the high-k layer. Such concentration of Al atoms at the high-k/SiO\textsubscript{2} interface may control the effective work function for PMOS devices. We note that inserting the AlO\textsubscript{x} layer also changes distribution of nitrogen atoms in the HfSiON layer. The total amount of nitrogen atoms decreases by AlO\textsubscript{x} layers. High nitrogen concentration in the high-k layer may be originated from the TiN gate electrode, so the insertion of AlO\textsubscript{x} layer prevents excess nitrogen diffusion from the electrode. Thus, it is found that effect of the AlO\textsubscript{x} capping layer at the interface of high-k/TiN strongly influences depth profile of nitrogen atoms [1].

**References**


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