Extended Abstracts of the 2011 International Conference on Solid State Devices and Materials, Nagoya, 2011, pp893-894

# Role of Al atoms in $(TaC)_{1-x}Al_x$ gate electrode on $V_{fb}$ for $HfO_2$ gate stack

M. Kimura[1], T. Nabatame[2], H. Yamada[1], A. Ohi[2], T. Chikyow[2] and T. Ohishi[1]

[1]Shibaura Institute of Technology, 3-7-5 Toyosu, Koto-ku, Tokyo 135-8548, Japan
Phone: +81-29-860-4915 E-mail: KIMURA.Masayuki@nims.go.jp
[2]MANA Foundry and MANA Advanced Device Materials Group,
National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan

## 1. Introduction

TiAlN and TaAlN gate electrodes have been investigated to control flatband voltage ($V_{fb}$) because of high work function ($\phi_m$) and dipole due to $AlO_x$ layer formation at high-k/$SiO_2$ interface for Hf-based high-k pMOSFET [1, 2]. On the other hand, nitrogen-free TaC has emerged as a promising gate electrode because of high mobility and thermal stability [3-5]. However, effect of Al atoms in Al-incorporated TaC ($(TaC)_{1-x}Al_x$) gate electrodes on $V_{fb}$ has not been understand yet.

In this paper, role of Al atoms in $(TaC)_{1-x}Al_x$-gated MOS capacitors with $HfO_2$ dielectric on $V_{fb}$ shift has been systematically studied with annealing temperature.

## 2. Experimental procedure

Multiple $(TaC)_{1-x}Al_x$-gated MOS capacitors were prepared as follows: A 4.2-nm-thick $HfO_2$ film was fabricated on $SiO_2$ (3 nm)/p-Si by MOCVD process. Typically, several 150-nm-thick $(TaC)_{1-x}Al_x$ films of various compositions (x = 0 - 0.33) were deposited on the $HfO_2$ film by sputtering method using TaC and Al metal targets. The post metal gate electrode deposition annealing (PMA) was varied from 500 to 1000 °C in $N_2$ after FGA at 400 °C in 3% $H_2$. To discuss bottom interface dipole, ALD-$Al_2O_3$ (3.4 nm) MOS capacitors with TaC and $(TaC)_{0.9}Al_{0.1}$ gate electrodes were also prepared. The $V_{fb}$ value was estimated from the C-V characteristics using the program MIRAI-ACCEPT [6].

## 3. Results and Discussion

### *3.1 A negative $V_{fb}$ shift in the low temperature region*

We first examined the structural properties in $(TaC)_{1-x}Al_x$ films. **Fig. 1** shows the typical XRD patterns of $(TaC)_{1-x}Al_x$ films after FGA. The face center cubic (FCC) structure of TaC was defected and the lattice constant shows almost same value in all compositions. The resistivity with Al content in $(TaC)_{1-x}Al_x$ films after annealing at 500 - 1000 °C are shown in **Fig. 2**. Note that the resistivity of $(TaC)_{1-x}Al_x$ films is almost unchanged in all ranges regardless of annealing temperature.

Relationship between $V_{fb}$ and Al content of the $(TaC)_{1-x}Al_x$-gated MOS capacitors with $HfO_2$ dielectric after FGA and PMA at 500 - 700 °C are shown in **Fig. 3**. The C-V curves shift to a more negative value as the Al content in the $(TaC)_{1-x}Al_x$ gate electrodes increases after FGA, as shown in an inset graph. A negative $V_{fb}$ shift occurs in all temperature ranges. This suggests that the $\phi_m$ of $(TaC)_{1-x}Al_x$ gate electrode changes lower by introducing Al atoms with a low $\phi_m$ (4.06 - 4.28 eV).

### *3.2 A positive $V_{fb}$ shift in the high temperature region*

Next annealing temperature dependence of $V_{fb}$ was evaluated. The C-V characteristics of TaC and $(TaC)_{0.9}Al_{0.1}$-gated $HfO_2$ MOS capacitors after PMA at 500 - 1000 °C are shown in **Fig. 4(a)** and **(b)**, respectively. The C-V characteristics of $(TaC)_{0.9}Al_{0.1}$-gated MOS capacitors significantly shift in the positive direction at above 800 °C, while the TaC-gated MOS capacitors show almost same profiles. The $V_{fb}$ behaviors of $(TaC)_{1-x}Al_x$-gated MOS capacitors are summarized in **Fig. 5**. We found that the direction of $V_{fb}$ shift changes according to annealing temperature. Note that the negative and positive $V_{fb}$ shifts as a function of x value occur at below 700 °C and above 800 °C, respectively. However, the x value is limited to less than 0.1 at above 700 °C because of a high leakage current.

### *3.3 Role of Al atoms in $(TaC)_{1-x}Al_x$ gate electrode on $V_{fb}$*

We expect that the positive $V_{fb}$ shift occurs by the $\phi_m$ change in $(TaC)_{1-x}Al_x$ gate electrode and/or bottom interface dipole formation due to $AlO_x$ layer grown at $HfO_2/SiO_2$ interface during PMA at high temperature. $Al_2O_3$ dielectric is employed to eliminate the influence of the dipole due to $AlO_x$ layer. The $V_{fb}$ changes of $Al_2O_3$ MOS capacitors with TaC and $(TaC)_{0.9}Al_{0.1}$ gate electrodes are shown in **Fig. 6**. It is clear that a positive $V_{fb}$ shift in $(TaC)_{0.9}Al_{0.1}$ gate electrode significantly appears at above 800 °C, while TaC gate electrode is almost unchanged. This indicates that the $V_{fb}$ shift is due to the $\phi_m$ change of $(TaC)_{0.9}Al_{0.1}$ gate electrode. Moreover, this suggests that Al content in $(TaC)_{0.9}Al_{0.1}$ gate electrode decreases because Al atoms of the gate electrode start diffusing into $HfO_2$ film at 800 °C. The $V_{fb}$ behaviors of $(TaC)_{0.9}Al_{0.1}$ gate electrode on $HfO_2$ film as a function of annealing temperature is shown in **Fig. 7**. The origin of $V_{fb}$ shift can be divided into two components such as $\phi_m$ of $(TaC)_{0.9}Al_{0.1}$ gate electrode and bottom interface dipole formation due to $AlO_x$ layer grown at $HfO_2/SiO_2$ interface. Note that effect of the dipole on $V_{fb}$ shift appears at above 900 °C. **Figure 8** is a schematic explanation of the role of Al atoms in $(TaC)_{1-x}Al_x$ gate electrode on $V_{fb}$ shift against annealing temperature. In the low temperature region below 700 °C, the effect of Al content on $V_{fb}$ significantly appears. At above 800 °C, the $\phi_m$ of $(TaC)_{1-x}Al_x$ gate electrode becomes higher because Al atoms diffuse into $HfO_2$ film. Finally, the $AlO_x$ layer, which is formed at $HfO_2/SiO_2$ interface at above 900 °C, induces the bottom interface dipole.

## 4. Conclusions

We investigated $V_{fb}$ behavior of $(TaC)_{1-x}Al_x$ gate electrode as a function of annealing temperature for $HfO_2$ MOS capacitors. The FCC structure and resistivity of $(TaC)_{1-x}Al_x$ films are almost unchanged regardless of x value in all temperature regions. We found that role of Al atoms in $(TaC)_{1-x}Al_x$ gate electrode on $V_{fb}$ changes according to annealing temperature. In the low temperature region below 700 °C, Al (low $\phi_m$) content causes a negative $V_{fb}$ shift. In contrast, in the high temperature region above 800 °C, Al content reduction in $(TaC)_{1-x}Al_x$ gate electrode and dipole formation due to $AlO_x$ layer grown by diffusing Al atoms into $HfO_2$ film lead to a positive $V_{fb}$ shift.

## References


[1] S. Jeon et al., *J. The Electrochem. Soc.* **157**, 1101(2010).
[2] M. Kadoshima et al., *IEDM Tech. Dig.* (2007) p.531.
[3] J. K. Schaeffer et al., *J. Appl. Phys.* **101**, 014503(2007).
[4] W. Mizubayashi et al., *VLSI Tech. Dig.* (2008) p.42.
[5] P. Homhuan et al., *Ext. Abs. IWDTF* (2011) p.9.
[6] N. Yasuda et al., *Ext. Abs. SSDM* (2005) p.250.


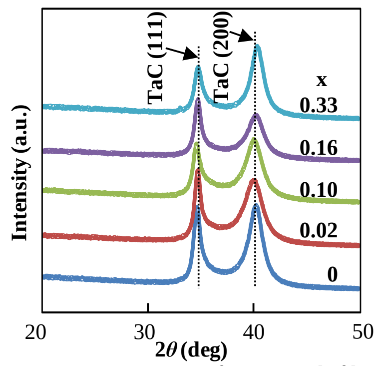


**Fig. 1.** XRD patterns of $(TaC)_{1-x}Al_x$ films after FGA at 400 °C in 3% $H_2$. All films consist of FCC structure of TaC and show almost same lattice constant.

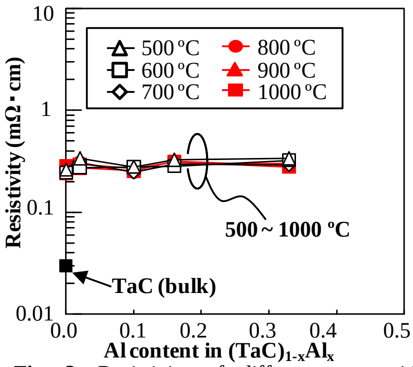


**Fig. 2.** Resistivity of different composition $(TaC)_{1-x}Al_x$ films as function of x value after PMA at 500 - 1000 °C. Resistivity of all films is almost unchanged in all PMA temperature.

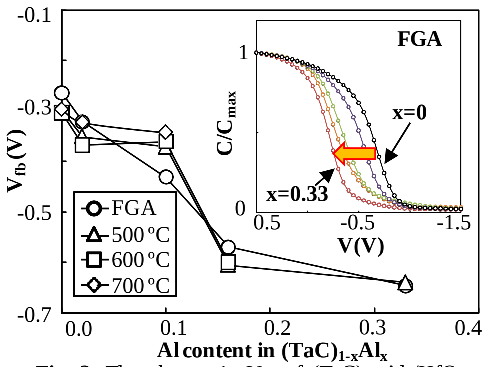


**Fig. 3.** The change in $V_{fb}$ of $(TaC)_{1-x}Al_x/HfO_2$ (4.2 nm) MOS capacitors against x value after PMA at 500 - 700 °C. An inset graph shows C-V curves after FGA. A negative $V_{fb}$ shift appears.

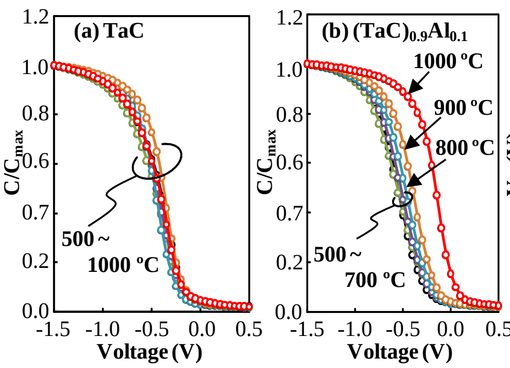


**Fig. 4.** The C-V characteristics of $HfO_2$ MOS capacitors with TaC and $(TaC)_{0.9}Al_{0.1}$ gate electrodes, respectively, after PMA at 500 - 1000 °C. The C-V curves of $(TaC)_{0.9}Al_{0.1}$ samples shift towards positive direction at above 800 °C, while the C-V curves of TaC samples are almost unchanged.

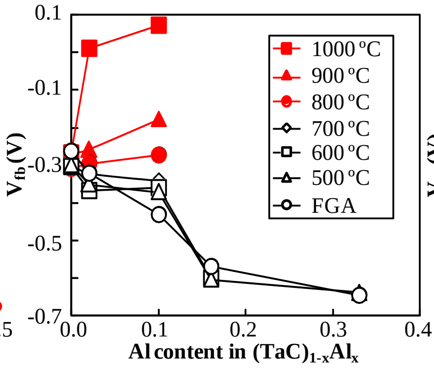


**Fig. 5.** The $V_{fb}$ change as a function of x value of $(TaC)_{1-x}Al_x$ gate electrodes after PMA at 500 - 1000 °C. A negative $V_{fb}$ shift appears below 700 °C and a positive $V_{fb}$ shift appears above 800 °C.

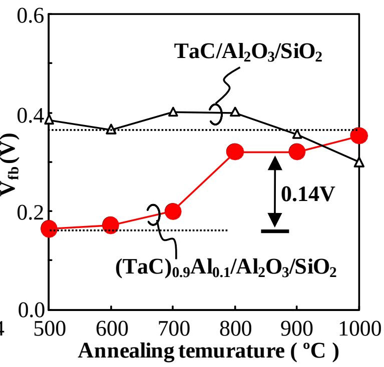


**Fig. 6.** The $V_{fb}$ change of $Al_2O_3$ MOS capacitors with TaC and $(TaC)_{0.9}Al_{0.1}$ gate electrodes as a function of PMA temperature. $(TaC)_{0.9}Al_{0.1}$ gate shows a positive $V_{fb}$ shift at above 800 °C.

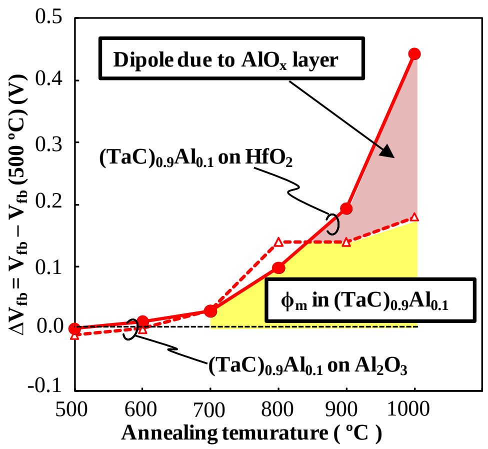


**Fig. 7.** Relationship between $V_{fb}$ shift and PMA temperature of $(TaC)_{0.9}Al_{0.1}$-gated MOS capacitors with $Al_2O_3$ and $HfO_2$ films. The origin of $V_{fb}$ shift is due to $\phi_m$ change in $(TaC)_{0.9}Al_{0.1}$ at above 800 °C and dipole formation of due to $AlO_x$ layer at above 900 °C.

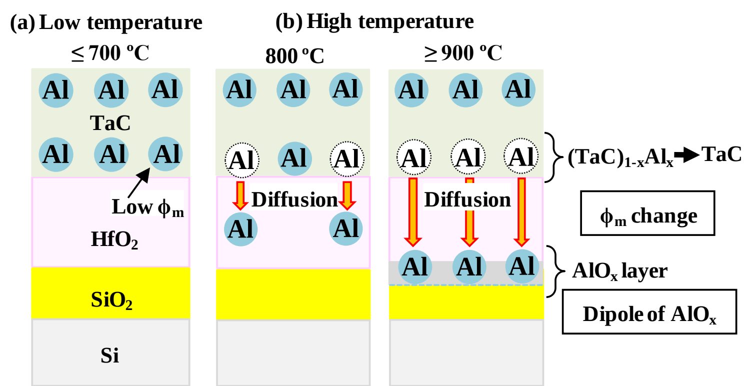


**Fig. 8.** Schematic explaining the role of Al atoms in $(TaC)_{1-x}Al_x$ gate electrode on $V_{fb}$ shift against annealing temperature. At below 700 °C, Al content in $(TaC)_{1-x}Al_x$ film causes a negative $V_{fb}$ shift. At 800 °C, Al content in $(TaC)_{1-x}Al_x$ film decreases because Al atoms diffuse into $HfO_2$ film. At above 900 °C, the dipole occurs because $AlO_x$ layer is formed at $HfO_2/SiO_2$ interface.