

# Characteristics and Mechanism of Tunable Work Function Gate Electrodes Using a Bilayer Metal Structure on SiO<sub>2</sub> and HfO<sub>2</sub>

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**Abstract**—In this letter, we investigate a method to adjust the gate work function of an MOS structure by stacking two metals with different work functions. This method can provide work function tunability of approximately 1 eV as the bottom metal layer thickness is increased from 0 to about 10 nm. This behavior is demonstrated with different metal combinations on both SiO<sub>2</sub> and HfO<sub>2</sub> gate dielectrics. We use capacitance–voltage (*C–V*) characteristics to investigate the effect of different annealing conditions and different metal/metal bilayer couples on the work function. By comparing the as-deposited and annealed films, and by comparing with metals that are relatively inert with each other, we deduce that the work function tuning behavior likely involves metal/metal interdiffusion.

**Index Terms**—HfO<sub>2</sub>, high- $\kappa$  dielectrics, metal gate, SiO<sub>2</sub>, work function.

## I. INTRODUCTION

AS CMOS technology continues to scale, metal gate electrodes need to be introduced to overcome the deleterious effects of doped polysilicon, namely gate electrode depletion, high resistance, and incompatibility with high- $\kappa$  gate dielectrics. In order to optimize low threshold voltage devices, metal gate electrodes will require work functions that can be tuned to a desired value. Many approaches including implanted metals [1], fully silicided gates [2], and alloy metals [3] have been studied in an effort to achieve tunable work function metal gates. Recently, the use of metal bilayers has been reported as another method to set the work function [4]–[7]. Here the work function is continuously changed from that of one metal to the other by changing the thickness of the bottom metal layer. Several bilayer metal

structures including Al/Ni [4], [5], Al/TaN [6], Ti/Pt and Ti/TiN [5], [7] have been fabricated on SiO<sub>2</sub> to achieve work function tuning. Several mechanisms were proposed to explain how the work function is changed in the bilayer stacks, including carrier redistribution [4], [6] and metal islanding of the thin film [7].

In this letter, we report on the use of a bilayer metal structure to tune the work function over a range of  $\sim 1$  eV with a variety of metals on SiO<sub>2</sub> and HfO<sub>2</sub> dielectrics. From the work function characteristics of as-deposited and annealed samples, a diffusion mechanism is proposed to explain the work function change as a function of bottom metal thickness.

## II. EXPERIMENT

MOS capacitors were fabricated on (100) Si wafers with thermally grown SiO<sub>2</sub> or metal–organic chemical vapor deposition HfO<sub>2</sub> of varying gate dielectric thickness. For the gate electrode, two metals with different work functions were deposited sequentially to form a bilayer structure. The metals were deposited by E-beam evaporation (unless otherwise specified) with the bottom layer thickness varying from approximately 1.5 to 10 nm and the top layer thickness being at least 30 nm. Samples with single layers of each of the two metals were also fabricated. After plasma gate etch, the gate stacks were subjected to a forming gas anneal (FGA) at temperatures up to 400 °C. The flat-band voltage,  $V_{fb}$ , was extracted from the capacitance–voltage (*C–V*) characteristics based on the NCSU *C–V* program [8] and plotted against the effective oxide thickness (EOT) to determine the work function for a range of gate metal thickness [9].

## III. RESULTS AND DISCUSSION

Fig. 1(a) shows the work function versus bottom layer (Pt) thickness after a 300 °C FGA for a Ti/Pt/SiO<sub>2</sub> bilayer electrode structure. It is clearly seen that the work function shifts from that of Ti ( $\Phi_m \approx 3.9$  eV) to that of Pt ( $\Phi_m \approx 5.3$  eV) as the Pt thickness is increased from 0 to  $\sim 6$  nm. We have also investigated Al/Ni/SiO<sub>2</sub>, Ti/W/SiO<sub>2</sub>, and Ta/TaN/SiO<sub>2</sub> structures. In all of these systems, a similar gradual work function transition is observed; at least 6 nm of bottom layer metal is required to change the work function from that of one metal to the other. Our results are consistent with reports of other bilayer systems such as Al/TaN [6], Pt/TiN, and Ti/TiN [7] on SiO<sub>2</sub>. The bilayer structure was also investigated on HfO<sub>2</sub> using Ti/Pt and Pt/Ti stacks as the gate electrodes. The work function dependence on the

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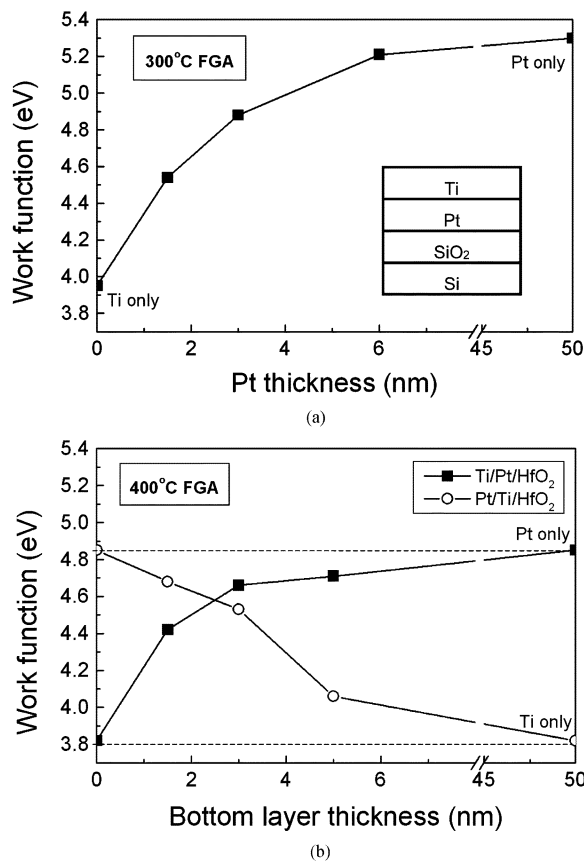


Fig. 1. (a) Work function versus Pt thickness for Ti/Pt/SiO<sub>2</sub> electrode stacks after 30 min, 300 °C FGA. (b) Work function versus bottom layer thickness for Ti/Pt/HfO<sub>2</sub> and Pt/Ti/HfO<sub>2</sub> electrode stacks after 30 min, 400 °C FGA.

bottom layer thickness after 400 °C FGA is shown in Fig. 1(b). The gradual work function transition observed for both stacks is very similar to that observed on SiO<sub>2</sub>. The difference in the work functions for the SiO<sub>2</sub> stack compared to the HfO<sub>2</sub> stack may be due to a Fermi level pinning effect in high- $\kappa$  dielectrics [10] and/or a reaction between the metal and HfO<sub>2</sub> [11]. Rather than an electrical or a discontinuous layer mechanism, atomic diffusion is more likely to explain the relatively large transition region of at least 6 nm. In all bilayer stacks we studied, a change in the work function behavior is observed before and after FGA. For example, for Ti/W on SiO<sub>2</sub>, the flat-band voltage [Fig. 2(a)] and the work function [Fig. 2(c)] of the as-deposited samples change abruptly, requiring 2.5 nm or less W in the bilayer to achieve the W work function. However, after a 400 °C FGA, a more gradual transition in the work function occurs with over 10 nm being required to reach the W work function value. These results imply that thermally activated diffusion is responsible for the work function shift rather than an electronic mechanism. The gradual transition in the work function can be explained by the diffusion of the top metal (Ti) atoms through the bottom metal (W) to the metal/dielectric interface during the annealing process. Another indication that Ti is at the interface is that an increase in accumulation capacitance is observed with decreasing W thickness [Fig. 2(b)]. This capacitance increase could be associated with Ti diffusing to the dielectric interface that reduces the interfacial SiO<sub>2</sub> resulting in a drop in EOT and an increase in capacitance [11].

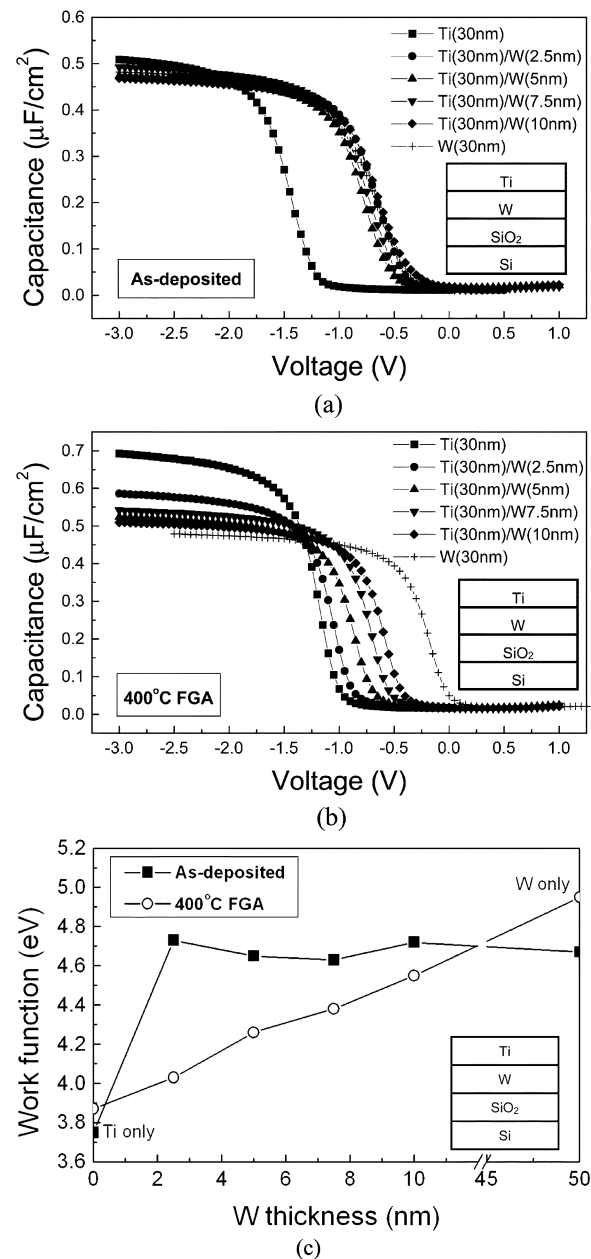


Fig. 2. High-frequency C-V characteristics of Ti/W/SiO<sub>2</sub> gate stacks (a) as-deposited and (b) after 30 min, 400 °C FGA (c) work function versus W thickness for as-deposited and after 30 min, 400 °C FGA Ti/W/SiO<sub>2</sub> gate stacks.

Several mechanisms have been proposed to explain this gradual work function change. The carrier redistribution mechanism has been reported [4], [6] to explain the observed behavior, but *ab initio* simulations of bilayer stacks [12] show that the transition of the work function should occur over the first 1–3 monolayers rather than the 6 nm or more observed experimentally. Metal islanding in ultrathin bottom layers was also hypothesized to explain this effect [7]. However, in our samples continuous bottom layers are observed in high resolution TEM images [5], and the gradual work function variation is still seen.

An additional approach to test the hypothesis that the change in work function with bottom layer thickness is a result of

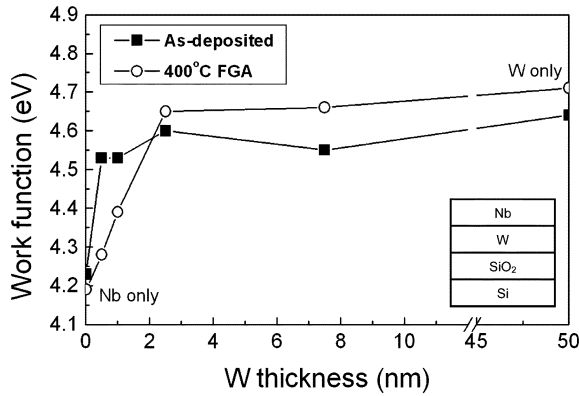


Fig. 3. Work function versus  $W$  thickness for Nb/W/SiO<sub>2</sub> gate stacks as-deposited and after 30 min, 400 °C FGA.

diffusion is to select two refractory metals, Nb and W, which, according to X-ray diffraction and diffusion data [13], undergo minimal interdiffusion and do not react in the temperature range we investigated. The other systems studied would be expected to exhibit appreciably higher interdiffusion based on their lower solidus temperatures [14]. For example, DiBattista and Schwank [15] examine diffusion of Ti in Pt thin films and report a range of diffusivities which are reasonably consistent with the diffusivity of  $\sim 2 \times 10^{-17} \text{ cm}^2\text{s}^{-1}$  we extract from the diffusion lengths associated with the gradual transition observed in the work function measurements. Measurements in the Nb/W system show a diffusivity of around  $10^3$  times smaller [13]. Fig. 3 shows the change in work function as a function of bottom layer thickness extracted from the  $C$ - $V$  characteristics of Nb/W/SiO<sub>2</sub> samples as-deposited (by sputtering) and after FGA (400 °C, 30 min). For the as-deposited case, a thin bottom layer of  $\sim 1$  nm is sufficient to change the work function from one metal to the other, which is consistent with the *ab initio* simulations [12] mentioned earlier. For the annealed samples,  $\sim 2$  nm of  $W$  is sufficient to change the work function from Nb to that of  $W$ , indicating some minimal intermixing. This degree of intermixing is somewhat larger than what might be expected based on the published diffusion coefficient [13], but still gives a more abrupt transition than other annealed samples [Figs. 1 and 2(c)]. These results for a minimally diffusing system support the model that a gradual transition in the work function as a function of bottom layer thickness, beyond a few monolayers, is due to diffusion rather than an electrical mechanism.

If diffusion is the mechanism, then this may have implications for device and reliability issues. For example, unequal diffusion of the species could lead to void formation, resulting in higher contact resistance or strain effects.

#### IV. CONCLUSION

We have demonstrated that the metal/metal bilayer structure can be used to adjust the gate electrode work function over a 1 eV range on both SiO<sub>2</sub> and HfO<sub>2</sub> dielectrics for a variety of

metals by controlling the thickness of the bottom metal layer. We propose that a possible mechanism for this behavior is the interdiffusion of the two metals. For combinations of metal/metal bilayers such as Al/Ni, Pt/Ti, and Ti/W, a gradual change in work function is observed for annealed stacks. However, for a system such as Nb/W in which interdiffusion is minimal the work function changes more abruptly thus confirming diffusion as a potential mechanism for the observed bilayer behavior.

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