Origins for Fermi level control in metal/high-k/Si stacks with inserted dielectric layers

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Controlling the metal's Fermi level position or the gate's effective work function (EWF) is an important aspect of advanced high-k/metal gate MOS devices. The prominent route to achieve this goal is the application of ultrathin dielectric layers, typically at the metal/high-k interface.

In a previous work we have found that the formation of a thin Ta sub-oxide layer at the Ta/Al_2O_3 interface created a dipole that increased the EWF [1]. Inspired by this result, the electrostatics of thin Ta_2O_5 layers were studied in Al_2O_3 based stacks, by varying the position of Ta_2O_5. A systematic analysis of the electrical characteristics revealed that Ta_2O_5 did not contribute any significant dipoles or fixed charges to the EWF. Instead, it was found that Ta_2O_5 could be used to inhibit the known dipole at the contact of Al oxide with SiO_2 [2] (Fig. 1). Given its high dielectric constant (~22), thin Ta_2O_5 provides an additional scalable degree of freedom for controlling the EWF.

In advanced commercial devices ultrathin capping layers are typically grown on top of the most common high-k dielectric, HfO_2. Two of the most studied dielectric caps for HfO_2 are oxides of Al and of La for increasing and decreasing the EWF, respectively. Even though the mechanism for the shift is still under debate [3], it is generally accepted that it is due to the presence of the cap's atoms at the dielectric/semiconductor interface. This interface often includes extremely thin Si oxide layers. Although the diffusion of La atoms has been studied in such a scenario [4], little is known about the diffusion of Al in the MOS stack.

HfO_2 MOS devices were fabricated with a varying position of a thin Al_2O_3 layer, at the top, middle or bottom of the HfO_2. The devices were subjected to low (400°C) and high (1000°C) temperature anneals. Our results show that at low temperatures Al_2O_3 has to be at the bottom of the dielectric, at its interface with SiO_2, in order to increase the EWF. By contrast, at high temperatures, all samples containing Al_2O_3 exhibited a EWF increase, and the closer the initial Al_2O_3 position to the bottom interface, the higher the EWF was (Fig. 2). To complement this indirect evidence of Al diffusion, a combination of ToF-SIMS and TEM analyses directly showed the diffusion of Al towards the bottom HfO_2 interface with SiO_2 and the accumulation of small quantities of Al there [5] (Fig. 3).

In order to compare La_2O_3 to Al_2O_3 capping, La_2O_3-capped HfO_2 stacks were fabricated, using a relatively thick, 7 nm, bottom SiO_2 (compared to a typical technologically-relevant value of ~0.5 nm). We compared the diffusion of La versus Al in the same configuration at low and high temperatures. The results showed that unlike the interfacial accumulation of Al, the La atoms were not stopped at the HfO_2/SiO_2 interface, but were rather incorporated inside the SiO_2 all the way to its interface with Si.

Several theoretical explanations were suggested for the mechanism of the opposite electrical effect of Al and La [3]. These theories revolved around the HfO_2/SiO_2 interface, where we have found the accumulation of Al. Our findings imply that the materials properties of the cap's atoms play a crucial role in its behavior during a high temperature anneal, and especially their different positions in the stack. While Al functions at the HfO_2/SiO_2 interface, in agreement with the current explanations, in the case of La one may consider creation of new or change of existing dipoles at the SiO_2/Si interface. This could further explain why another rare-earth element, Gd, that is also reactive with SiO_2, has a similar effect to La, of lowering the EWF.

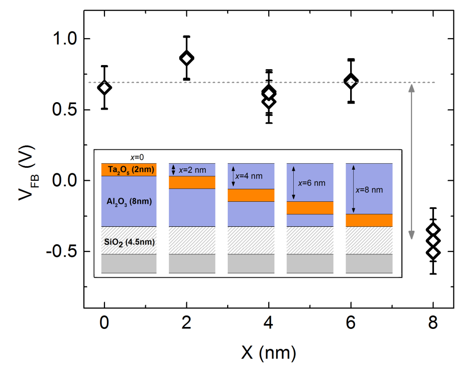

Figure 1. Flat band voltages versus the Ta_2O_5 position, X, that is illustrated in the inset [2].

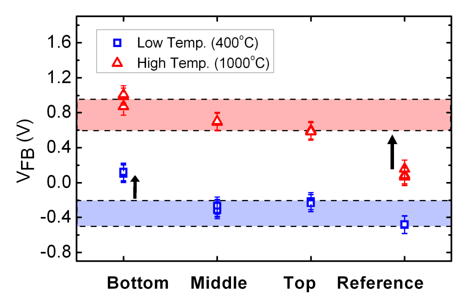

Figure 2. Flat band voltages versus the Al_2O_3 with respect to HfO_2 at low and high anneal temperatures [5].

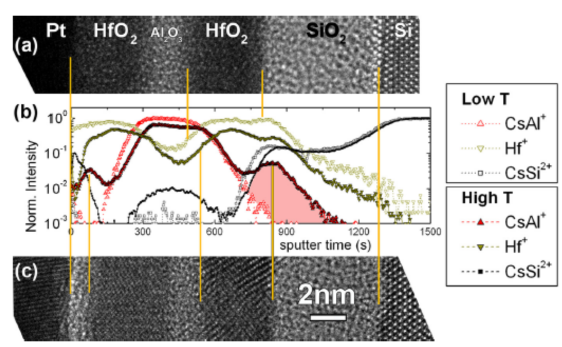

Figure 3. Cross section TEM micrographs of (a) low- and (c) high temperature annealed "middle" sample versus (b) the elemental distribution obtained with ToF-SIMS [5].

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