Origins for Fermi level control in metal/high-k/Si stacks with inserted dielectric layers
Moshe Eizenberg and Lior Kornblum
Dept. of Materials Science & Engineering, Technion – Israel Institute of Technology
Haifa 32000, Israel

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 interface created a dipole that increased the EWF [1]. Inspired by this result, the electrostatics of thin TaOx layers were studied in AlOx based stacks, by varying the position of TaOx. A systematic analysis of the electrical characteristics revealed that TaOx did not contribute any significant dipoles or fixed charges to the EWF. Instead, it was found that TaOx could be used to inhibit the known dipole at the contact of Al oxide with SiO2 [2] (Fig. 1). Given its high dielectric constant (~22), thin TaOx 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, HfO2. Two of the most studied dielectric caps for HfO2 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 observed and studied in such a scenario [4], little is known about the diffusion of Al in the MOS stack.

HfO2 MOS devices were fabricated with a varying position of a thin AlOx layer, at the top, middle or bottom of the HfO2. The devices were subjected to low (400°C) and high (1000°C) temperature anneals. Our results show that at low temperatures AlOx has to be at the bottom of the dielectric, at its interface with SiO2, in order to increase the EWF. By contrast, at high temperatures, all samples containing AlOx exhibited an EWF increase, and the closer the initial AlOx 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 HfO2 interface with SiO2 and the accumulation of small quantities of Al there [5] (Fig. 3).

In order to compare LaOx to AlOx capping, La2O3-capped HfO2 stacks were fabricated, using a relatively thick, 7 nm, bottom SiO2 (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 HfO2/SiO2 interface, but were rather incorporated inside the SiO2 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 HfO2/SiO2 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 HfO2/SiO2 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 SiO2/Si interface. This could further explain why another rare-earth element, Gd, that is also reactive with SiO2, has a similar effect to La, of lowering the EWF.

References: