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On the role of Al doping at the SiO_2/HfO_2 interface ONISE SHARIA, A.A. DEMKOV, UT Austin, G. BERSUKER, B.H. LEE, SEMATECH —
One of the main challenges associated with the integration of high-k gate dielectrics such as hafnia is the identification of metal electrodes exhibiting the work function aligned with Si band edges. Due to the inherent instability of metals in contact with hafnia under high temperature, the focus has recently shifted towards developing a metal gate stack with appropriate effective work functions (EWF), which would result in the required low transistor threshold voltage. In this talk we report the theoretical results on doping the SiO_2/HfO_2 gate stack with Al atoms which, as we show, controls the EWF. We consider several dopant-vacancy models in various positions with respect to the interface. The proper stoichiometry avoiding fixed charge is maintained in all models. We find that doping at the interface has lower energy than doping in the bulk of silica or hafnia, which suggests the segregation of Al atoms towards the interface. Importantly, in all cases Al-vacancy complexes at the interface significantly change the band alignment, reducing the valence band offset. Thus, doping the SiO_2/HfO_2 gate stack with Al atoms offers a consistent way to adjust the alignment. This increase of the EWF can be explained with our previously introduced model that suggests that an oxygen depleted interface provides less effective screening, which in turn increases the interface dipole.

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