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Electronic properties and band alignments of Hf-based gate dielectrics on silicon R. PUTHENKOVILAKAM, J. CHOI, J.P. CHANG, Department of Chemical Engineering, University of California, Los Angeles — Ultra thin Hf-based dielectrics are being considered for possibly replacing SiO_2 gate oxide in silicon based metal- oxide-semiconductor (MOS) transistors. In this work we investigated the electronic structure and band alignments of the Hf-based gate dielectrics on silicon, which dictate the device performance of transistors in the sub-90nm devices. The electronic structure of HfO_2/Si interface showed dangling bond states at the interface due to the reduced coordination of Hf caused by the intrinsic bond constraints at the HfO_2/Si interface. However, our calculations indicate that these dangling bonds could be passivated by hydrogen or oxygen, which can appropriately change the coordination numbers at the interface, thereby removing the dangling bond states. We also considered the interface of $HfSiO_4$/Si and found that there are no dangling bond states at the interface, making $HfSiO_4$ a promising interfacial layer to improve the interface quality. Band offsets at the interfaces with Si were calculated using density functional theory, and it showed that the band offsets vary depending upon the interface stoichiometry. Band alignments were also determined experimentally using XPS and were in excellent agreement with the theoretical results. Incorporation of nitrogen into the HfO_2 network resulted in notable changes in the valence band structure of the material and the corresponding band alignments with silicon and is found to depend on the nitrogen concentration in the bulk of HfO_2 as well as at the interface.

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