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The effect of Al content on the work function engineering at TiAlN/HfO_2 interface[1] GEUN-MYEONG KIM, YOUNG JUN OH, KEE JOO CHANG, Department of Physics, KAIST — In high-k/metal gate stacks of metal-oxide-semiconductor field-effect transistors, it is important to control the metal work function such that it should be close to the valence and conduction band edges of Si in p- and n-channel devices. It was reported that depositing TiAl on top of TiN/HfO_2 stack in gate-last process can effectively induce the n-type shift of work function, while the work function is of p-type at TiN/HfO_2 stack. In this work, we perform first-principles density functional calculations to investigate the Schottky barrier height at TiAlN/HfO_2 interface. In bulk TiN, it is found that a substitutional Al is the most stable form of Al impurity. When substitutional Al atoms are introduced at TiN/HfO_2 interface, the effective work function tends to decrease. At TiAlN/HfO_2 interface, the n-type shift of the work function increases almost linearly with the Al content. This is attributed to the change of interface bonds by Al incorporation and the dipole field induced at the interface. On the other hand, relative thicknesses of TiAl and TiN at abrupt TiAl/TiN/HfO_2 interface do not significantly affect the effective work function.

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