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The effect of Si impurities on the effective work function at TiN/tetragonal-HfO_2 interface. GEUN-MYEONG KIM, YOUNG JUN OH, KEE JOO CHANG, Department of Physics, KAIST — The TiN/monoclinc-HfO_2 (TiN/m-HfO_2) interface structure is widely used in high-k/metal gate stacks of metal-oxide-semiconductor field-effect transistors. As the device size is continuously reduced, high-k dielectric materials are required to reduce the gate leakage current. The tetragonal HfO_2 (t-HfO_2) is beneficial in high-k/metal gate stacks because its dielectric constant is much higher than that of m-HfO_2. It is known that Si doping can reduces the crystalline temperature of t-HfO_2. However, there is a lack of studies for the effect of Si impurities at TiN/t-HfO_2 interface. Here we perform first-principles density functional calculations to investigate the effect of Si impurities on the work function at TiN/t-HfO_2 interface. It is energetically favorable for Si atoms to substitutes for interface N atoms. The change of interface bonds by the Si atoms enhances the effective work function(EWF). On the other hand, when the Si atoms replace the N atoms in bulk region, the EWF is almost unchanged. Our results indicate that the Si impurities incorporated in the interface region mostly affect the work function at TiN/t-HfO_2 interface.

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