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The electronic structure of O-vacancy at the interface between Si and HfO_2[1] BYUNGKI RYU, KEE JOO CHANG, Department of Physics, Korea Advanced Institute of Science and Technology — We study the electronic properties of oxygen vacancy (V_O) at the interface structure between Si and HfO_2 through local density functional calculations. We consider a device model, where HfO_2 layers are placed on the Si (001) surface. For monoclinic and amorphous HfO_2, the valence band offsets are estimated to be 2.0–3.0 eV. The defect properties of V_O are affected by the local bonding geometry and band offset at the interface. We find that V_O defects at the interface, which are surrounded by a mixture of the Hf and Si atoms, have lower formation energies than those in the oxide region. For various interface structures, we find that the defect levels of V_O are generally higher in the amorphous phase than in the monoclinic phase due to the smaller valence band offset. Our calculations suggest that the Fermi level pinning in p-MOS devices is caused by O-vacancies in the oxide region, more significantly in the amorphous oxide. On the other hand, O-vacancies formed at the interface, which have the unoccupied levels in the Si band gap, are responsible for the Fermi level pinning in n-MOS devices.

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