

Abstract Submitted
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Internal dielectric interface: SiO₂- HfO₂ ONISE SHARIA, ALEX DEMKOV, GENADI BERSUKER, BYOUNG HUN LEE — Hafnia is the leading candidate to replace silica as the gate dielectric in CMOS technology. Typically, hafnia films are deposited by atomic layer deposition (ALD) on the oxidized surface of a silicon wafer. The oxide could be native or thermally grown. Therefore, the high-k dielectric film is not in direct contact with Si, but rather with silicon dioxide. We investigate theoretically the atomic structure of the SiO₂-HfO₂ interface, its energetics, and thermodynamic stability with respect to oxygen exchange across the interface. We have examined the electronic properties of the interface including the band discontinuity using density functional theory. To model the interface we build a supercell structure by connecting β -cristobalite (crystalline silica polymorph) and cubic hafnia. This model, while being obviously rather simplistic allows for systematic study of the dielectric thickness effects, and consistent placement of defects with respect to the interface. The striking atomic feature of the calculated interface structure is three-fold coordinated interfacial oxygen atoms connected to one Si and two Hf neighbors. The Si-O and Hf-O bond lengths are 1.62 and 2.1 Å, respectively. The energy of the interface is estimated to be in the range of 900-4000 erg/cm² depending on the oxygen chemical potential. The structure has no states in the gap, and the estimated valence band offset agrees well with the MIGS theory. We discuss the effect of vacancies on the band alignment, and possible implications of our results to Si-SiO₂-HfO₂-Metal stacks.

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