

Abstract Submitted
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Segregation of O defects in Si:HfO₂ heterojunctions: A first principles investigation. R. RAMPRASAD, C. TANG, University of Connecticut — Driven by a need for device miniaturization in the microelectronic industry, Hf-based high-permittivity materials, such as HfO₂, have gained interest for their potential application as gate dielectrics. However, undesirable interfacial phases such as Hf silicides and SiO_x are known to form and degrade the performance of devices. It has been postulated that these interfacial phases are related to the segregation of O defects (vacancy or interstitial) to the interface. In this work, we examine the thermodynamic and kinetic driving forces for the segregation of isolated and clustered O defects (vacancies and interstitials) to the Si:HfO₂ interface. Using first principles density functional theory calculations, we have determined the formation and migration energies per O defect within bulk HfO₂ and at the Si:HfO₂ interface. Our results indicate that isolated as well as a distribution of point defects display large driving forces for interface segregation, allowing for the formation of silicides and silicates. Thus, while an abrupt Si:HfO₂ interface may be stable in the absence of O defects, such an interface is unstable to the formation of other phases in the presence of O defects.

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