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A first principles thermodynamic study of Si-HfO_2 and Pt-HfO_2 interfaces HONG ZHU, RAMPI RAMPRASAD, University of Connecticut — Atomic-level control of dielectric-semiconductor and dielectric-metal interfaces has become critical in determining the properties of the emerging high-k oxide-based MOSFETs. Using Si-HfO_2 and Pt-HfO_2 as an example, we investigate the evolution of these interface structures and electronic properties as a function of processing conditions by combining density functional theory results and statistical thermodynamics. Firstly, using first principles thermodynamics (FPTs), we determine the phase diagrams of Si-HfO_2 and Pt-HfO_2 interfaces. The vibrational and configurational entropic contributions to the free energies of the condensed phases are explicitly included. We demonstrate that the predictions of the FPT approach are in quantitative agreement with experiments for the interfaces considered. Secondly, a parameter-free methodology to determine the work function shift (or effective work function, EWF) of metal when interfaced with oxide is developed. This strategy is combined with statistical thermodynamics to predict the most probable EWF at given processing condition. The favorable agreement between the computed and experimental EWFs under generally adopted conditions is indicative of the usefulness of such full first-principles property-processing relationship studies.

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