289o Dft Calculations of Tio2 Atomic Layer Deposition

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Two of the most critical issues currently facing the semiconductor industry are the discovery of high-ê gate dielectric replacement materials for SiO2 and the development of deposition processes that will afford high surface uniformity and controlled growth at the atomic scale. Atomic layer deposition (ALD) is an ideal candidate for meeting these challenges, enabling the deposition of a material through highly uniform and conformal growth, with thickness control at the atomic layer level. Our current work involves the use of a multi-scale modeling strategy to gain theoretical insights into ALD at the atomic scale, as applied to the deposition of TiO2 thin films. First, information about the atomic processes and energetics involved is gathered using ab initio density functional theory (DFT) studies. Then, based on the results of the DFT calculations, the dominant kinetic processes occurring on the surface can be modeled simultaneously using the Kinetic Monte Carlo (KMC) simulation technique. This technique provides information about the kinetics of the processes occurring on the surface, while preserving the essential atomic structural details of the system. Based on these muti-level simulations, a better understanding of the mechanisms and the critical factors contributing to the ALD film growth process can be obtained. In this work, we present results from the first phase of our simulation strategy, which involves ab initio calculations of TiO2 film growth from TiCl4 and H2O precursors on a hydroxylated SiO2 substrate. A series of cluster calculations were carried out to study the atomistic mechanism and energies of the elementary reactions of the two deposition half-cycles. The potential energy surface and Gibbs free energy surfaces are predicted at three typical growth temperatures. In conjunction, the temperature dependence of the film growth are discussed. As far as we know, this is the first ab initio investigation of this system, despite its relevance to the semiconductor industry. We also plan to expand our work in the future by investigating bulkier metal precursors, such as TiI4 and titanium alkoxydes, in order to understand the effect of steric hindrance during the deposition process.