

Sequential removal of ligands from  $\text{TiCl}_4$  on  $\text{SiO}_2$  surface during atomic layer deposition: a DFT study

박정우, 문지원<sup>1</sup>, 진유성<sup>1</sup>, 박형순<sup>1</sup>, 정성웅<sup>1</sup>, 송봉근<sup>†</sup>  
홍익대학교; <sup>1</sup>SK hynix  
(bshong@hongik.ac.kr<sup>†</sup>)

Atomic layer deposition (ALD) is a thin film deposition technique that can produce uniform and conformal thin films with atomic thickness control on nanostructured substrate. It is known that the adsorption chemistry of the metal precursors on the substrate surface can be a crucial factor for uniformity of the deposited materials. Here, we present a periodic dispersion-corrected density functional theory (DFT) study of sequential dissociation reactions of the Cl ligands from the titanium tetrachloride ( $\text{TiCl}_4$ ) precursor on  $\text{SiO}_2$  surface. As a model substrate, a fully hydroxylated  $\alpha$ -quartz (001) surface was considered. It is shown that removal of first three Cl ligands are feasible with small thermal activation, leading to adsorbed \*Ti-Cl and generating gaseous HCl byproducts. However, removal of the fourth Cl ligand involve large activation barrier over 10 eV and endothermicity of ca. 5 eV, suggesting removal of Cl ligands during adsorption of  $\text{TiCl}_4$  will be incomplete. Our study suggest that the chemical aspects of the ALD process can be analyzed utilizing quantum mechanical simulations.