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Multi scale modeling of atomic layer deposition[1]
MAHDI SHIRAZI, SIMON D. ELLIOTT, Tyndall National Institute
— Atomic layer deposition (ALD) is one of the techniques now used to grow conformal nanometer thin films with the quality required for electronic devices. ALD is a type of chemical vapor deposition that depends on self-limiting surface chemistry. Many aspects of chemical reactions and their effect on the stoichiometry of the film remain unclear. We have used therefore density functional theory (DFT) to explore those reactions. The growth of HfO_2 from H_2O and $Hf(N(CH_3)_2)_4$ was regarded as a sample ALD system. The process of densification was explained accurately. A new mechanism of multiple proton diffusion was propounded and DFT energetics showed it to be the most favourable path way. We also found that reaction rates are strongly coupled with the coordination number of Hf atoms at the surface. Then this complex chemistry was implemented in kinetic Monte-Carlo (KMC). The KMC calculation showed the effect of intermediate reactions on the growth rate. Furthermore the morphology of the film and the growth rate under different reaction conditions were compared with experimental data.

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Mahdi Shirazi
Tyndall National Institute

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