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Density Functional Theory Simulations of Atomic Layer Deposition of HfO2 JOSEPH HAN[1], Stanford University, CHARLES MUSGRAVE, Stanford University — We have used DFT to predict the growth mechanisms and kinetics of hafnium oxide ALD using metal chloride and metal alkylamide precursors. We have determined parameters for Arrhenius rate equations and compare with experimental results to propose explanations for the different observed film growth characteristics including submonolayer deposition, non-uniform growth, and impurity incorporation. We find that in the case of Hf tetrachloride, etching reactions are significant and lead to film defects. Furthermore, HfCl4 ALD reactions have relatively high barriers which necessitate the use of high ALD temperatures. However, in contrast to the metal chloride system, we predict kinetics that suggest that deposition process using alkylamine precursors should occur at lower temperatures with better growth characteristics, such as a more uniform film with less impurity incorporation.

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