Monte Carlo Simulation in a Laptop for Understanding Physical Interaction of Atomic Layer Deposition Precursors

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Since the reaction of atomic layer deposition (ALD) strongly depends on surface property, understanding of surface reaction mechanism between substrates and precursors is essential to predict and interpret thin film deposition in ALD. Recently, the many researchers have studied chemical reactions of ALD using density functional theory (DFT) and physical reaction using molecular dynamic (MD). However, DFT is suit for calculating a few of molecule adsorption but not simultaneous multiple adsorptions, and MD is not proper for a large scale simulation due to huge computing resource and long calculation time. In addition, although the steric hindrance effect between the molecules is an important physical factor for simulation of ALD, but it was not considered as a main variable for simulation. In this study, by adopting several assumptions and approximations, we developed a simple simulation method to understand physical steric hindrance effects of ALD precursors by using Monte Carlo (MC) without huge computing resources and applied the method to study surface reaction mechanism of ALD and area selective ALD (AS-ALD). We calculated the areal coverage of precursor on a specific surface used in ALD and AS-ALD using the MC simulation with a random adsorption model. The simulation results show high consistency agreement with experiment data. Based on the 2D model developed first, we extended the MC simulation to 3D system, and obtained reliable results in bulky precursor systems. The simulation method developed in this study could be applied to many of ALD precursors and AS-ALD inhibitor systems just by using a laptop computer.