Computational Modeling of Physical Surface Reactions of Precursors in Atomic Layer Deposition by Monte Carlo Simulations

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The continuously increasing demand for down-scaling of devices in the semiconductor industry has increased the need for ultrathin films. Atomic layer deposition (ALD) is the most promising technique for this purpose and has attracted significant interest. Since ALD is based only on surface reactions of precursors and reactants, understanding the reaction mechanism of the precursor with the substrate surface is crucial. The surface reactions of ALD could be categorized into chemical reaction and physical reaction. The chemical reactions in ALD have been interpreted by adsorption energies of precursors and reactant calculated by the first principle method, density functional theory (DFT). However, the physical reactions of ALD precursors and reactants have not been studied using computational methods, such as molecular dynamics due to limitation in calculation size and computing resources. In this presentation, the ALD reaction mechanisms are investigated using Monte Carlo (MC) simulations based on a simple steric hindrance model. The physical surface reactions of the precursors are modeled using MC simulations, and the steric hindrance effect of precursor adsorption on surfaces is easily predicted using a laptop computer without requiring significant computing resources. The proposed MC simulation models yield highly consistent results with experimental data and theoretical results obtained from density functional theory calculations. We believe that this simulation method can be a useful tool with a laptop-scale computer for researchers and students working on understanding surface reactions of ALD.