Atomic Layer Modulation using Steric Hindrance of Precursors

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Atomic layer deposition (ALD) is a technique frequently used through the supercycle manner to fabricate multicomponent thin films. The stoichiometry of thin film can be controlled by changing the ratio of each ALD cycle. These days, most of applications require reduced film thickness with high stoichiometric uniformity in few nanometers. However, the conventional supercycle approach has limitations in reduction of thickness because it requires a certain thickness to achieve the desired stochiometric uniformity. In addition, the stoichiometric uniformity of the multicomponent ALD films does not well matched with the calculated value by the cyclic ratio due to unknown mixing mechanisms. In this work, we proposed a different approach by ALD using steric hindrance effects of precursors. Two precursors with different molecules size are sequentially exposed to the surface, and the stoichiometry of the film is determined and controlled by the adsorption coverage ratio of precursors based on steric hindrance of two precursors. The experiments were conducted using a ruthenium precursor, dicarbonyl-bis-(5-methyl-2,4-hexanediketonato)Ru(II) (Tanaka Kikinzoku Kogyo) with two Al precursors, trimethylaluminum (TMA) and dimethylaluminum isopropoxide (DMAI) (Lake Materials). The adsorption coverages by steric hindrance effects of precursors on the SiO_2 substrate surface were simulated by Monte Carlo (MC) method. The density functional theory (DFT) calculation was also performed to estimate the favorable adsorption of each precursor on the surface, supporting the experimental results and interpretation of atomic layer modulation (ALM) thin films. The theoretical calculation results were consistent with the analyzed stoichiometry of the films. The results in this work have a big potential to fabricate a nanometer-thick multicomponent ALM film for various applications.