Area-Selective Atomic Layer Deposition Al_2O_3 using a Small Thiol Inhibitor and Effects of Precursor size

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Area-selective atomic layer deposition (AS-ALD) is attracting increasing interest because of its ability to enable both continued dimensional scaling and accurate pattern placement for next-generation nanoelectronics. Self-assembled monolayers (SAM) have been used as inhibitor to change the surface property in AS-ALD. The conventional SAMs, however, were relatively long and big in the range of 2~3 nm, so they are not suit for AS-ALD in few nanometer scale 3D patterns. In this work, we investigated ethanethiol (ET) for a small size inhibitor of AS-ALD on metal substrates, Co and Cu. We used two Al precursors with different molecular size, trimethyl-aluminum (TMA) and dimethyl-aluminum-isopropoxide (DMAI) for blocking property, with H_2O counter reactant. ET was selectively absorbed on Cu and Co, but not on SiO_2 and showed better inhibition property against ALD Al_2O_3 using DMAI than that using TMA. In order to investigate the different blocking property of ET to TMA and DMAI, we calculated the adsorption kinetics and dynamics of Al precursors on Cu and Co surfaces inhibited by ET using density-functional theory (DFT) and realized physical adsorption behavior based steric hindrance using Monte-Carlo (MC) simulation. DFT results showed that DMAI forms dimers during adsorption on surfaces, and TMA preferably reacts even on the CH_3-terminted ET surfaces. Consistently, the steric hindrance simulation by MC showed a reasonable difference in Al precursor adsorptions on ET-inhibited Co and Cu surfaces. From the results and knowledge, we could extend the degree of freedom to obtain better AS-ALD property to selection of ALD precursors, and it could be applied to other AS-ALD materials systems.