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Atomistic simulations of plasma-surface interaction for ALD and ALE processes SATOSHI HAMAGUCHI, YUKI OKADA, MICHIRO ISOBE, TOMOKO ITO, KAZUHIRO KARAHASHI, Osaka Univ — Molecular dynamics (MD) simulation and quantum mechanical (QM) first-principles simulation are powerful tools to analyze complex surface reaction mechanisms of atomic layer deposition (ALD) and atomic layer etching (ALE) processes. For example, in ALE of SiO2 films, deposition of a few-angstrom deep fluorocarbon (FC) layer on a SiO2 film and a subsequent application of low-energy Ar+ ions to the fluorocarbon-deposited SiO2 film is known to cause sub-mono-layer etching of the SiO2 surface. MD simulation of such a process has shown that low-energy Ar+ ion bombardment causes a mixing of the FC layer with the underneath SiO2 surface as well as preferential sputtering of O atoms, resulting in the formation of a relatively Si-rich thin layer incorporating F and C atoms. In other words, Ar+ ion bombardment promotes two competing surface reactions: one is the formation of volatile SiFx moieties, which may lead to the desorption of surface Si atoms, and the other is the formation of a SiC network, which can hinder such desorption. For ALE of metal surfaces due to the formation of metal organic complexes, QM simulation can reveal energetically preferred surface reactions. Comparison of the simulation results with experimental observations for such processes will be also discussed.

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