Atomic Layer Etching
Room Arteveldeforum & Pedro de Gante - Session ALE-MoP
Atomic Layer Etching Poster Session

ALE-MoP-3 Density Functional Theory Study on the Reactions of Fluorine-Containing Molecules on Silicon Nitride Surface, ***Tanzia Chowdhury***, *R Hidayat, H Kim,* Sejong University, Republic of Korea*; T Mayangsari,* Universitas Pertamina, Indonesia*; S Park,* Wonik IPS, Republic of Korea*; J Jung, W Lee,* Sejong University, Republic of Korea

Silicon nitride is one of the most extensively used silicon-based materials in semiconductor devices. It has been used as gate spacers and diffusion barriers for many decades and was recently introduced to the charge trap layer and the sacrificial layers for three-dimensional (3D) NAND devices. The integration of silicon nitride into these devices often requires selective removal of silicon nitride against other materials, such as silicon oxide or silicon, and vice versa. With the continuing device miniaturization, atomic-scale processes such as atomic layer etching (ALE) has been developed for controlled removal of thin layers. ALE consists of the modification of the surface and the removal of the modified layer. The species used to modify the surface plays a crucial role in the overall process. The ALE of silicon nitride was reported by the modification by CH_3F gas adsorption and the removal of the modified layer by Ar ion bombardment [1]. However, the comparative study on the interaction of different gaseous fluorine-based molecules with the silicon nitride surface is yet to be presented. Ab initio atomic-scale simulation can be a convenient method to study the underlying surface chemistry as well as to outline new etching process routes. Previously, we modeled and simulated the initial fluorination reactions of SiO_2 and Si surfaces by various fluorine-containing gas molecules [2]. In the present study, density functional theory (DFT) calculations have been employed to investigate the initial reaction of fluorine-containing molecules on an NH_2 and NH-terminated Si3N4 surface. We chose a comprehensive set of hydrofluorocarbons and hydrogen fluoride, such as CF_4, CHF_3, CH_2F_2, CH_3F, and HF. Surface reaction mechanisms were studied by modeling and simulation of possible reaction pathways to determine the adsorption energy, activation energy, reaction energy, and desorption energy. Finally, we compared the reactions on the Si_3N_4 surface with the reactions on the OH-terminated SiO_2 and H-terminated Si surfaces.

References

[1] W.H. Kim et al., J. Vac. Sci. Technol. A, 36, 01B104 (2018)

[2] T. Chowdhury et al., J. Vac. Sci. Technol. A, 37, 021001 (2019)

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