Modeling of dry cleaning processes of semiconductor surfaces using fluorine-based etchant gases

Tanzia Chowdhury [1], Romel Hidayat [1], Tirta Rona Mayangsari [1], Jiyeon Gu [1], Hye-Lee Kim [1], Jongwan Jung [1], and Won-Jun Lee [1]

[1]Sejong Univ., Korea, Republic of

Introduction of 3D device architectures and scaling of device dimensions of integrated circuits inflict major challenges in modern semiconductor manufacturing technology. Formation of functional structures down to sub-10nm scale requires extremely smooth and clean surfaces. Utilization of the conventional wet cleaning processes has its limitation at this projected structural feature. Dry cleaning of semiconductor surfaces is considered to be a compelling technique as it demonstrates the multifaceted advantages over wet etching processes, such as the ability to access smaller structures and the absence of damage caused by surface tension. Fluorine-based molecules have been used for dry vapor phase etching of semiconductor surfaces and many experimental studies with varying process parameters have been conducted extensively. The underlying chemistry between etchants and surfaces are complex and requires profound exploration in the theoretical ground. Ab initio atomic scale simulation can be a convenient mean to interpret well established experimental techniques along with outlining new etching process routes. A detailed simulation study of reaction mechanism between etchants gases with various surfaces is yet inadequate in the literature.
In this study, density functional theory (DFT) calculations have been employed to investigate the effect of etching gases on different surfaces. The reaction in which the H-terminated Si or Ge surface or the OH-terminated SiO_2 or GeO_2 surface is fluorinated by a fluorine-based gas such as NF_3, ClF_3, CF_4 or CHF_3 is modeled and simulated by the DFT method. Surface reaction mechanisms were studied by the reaction energy and the energy barrier. A comprehensive understanding of the surface reactions during the dry cleaning process can provide valuable insights into the selective epitaxial growth process.

This work was supported by the Korea Institute of Energy Technology Evaluation and Planning(KETEP) and the Ministry of Trade, Industry & Energy(MOTIE) of the Republic of Korea (No.20172010106080).