PLASMA-SURFACE INTERACTIONS IN NANOSCALE PROCESSING: PRESERVATION OF LOW-*k* INTEGRITY AND HfO_2 GATE-STACK ETCHING WITH Si SELECTIVITY*

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Plasma-surface interactions are very important in the fabrication of the nm-sized features of integrated circuits. Plasma processes are employed to produce high-resolution patterns in many of the thin layers of silicon integrated circuits and to remove masking layers while maintaining high selectivity. Integrated plasma processes consisting of sequential steps such as etch, clean and surface modification, are used in semiconductor industries. The surface in contact with the process plasma is exposed to the fluxes of neutrals, ions, molecules, electrons and photons.

Modeling of surface reaction mechanisms requires the determination of the characterizations of fluxes (e.g. composition, magnitude, energy and angle) and development of the reaction mechanisms of the processes such as adsorption, reflection, bond breaking and etch product evolution, while reproducing the experimental results. When modeling the reaction mechanism for an entirely new material, the experimental data is often fragmentary. Therefore, fundamental principles such as bond energies and volatility of the etch products must be considered to develop the mechanism. In this thesis, results from a computational investigation of porous low-*k* SiCOH etching in fluorocarbon plasmas, damage during cleaning of CF_x polymer etch residue in Ar/O_2 and He/H_2 plasmas, NH_3 plasma pore sealing and low-*k* degradation due to water uptake, will be discussed. The plasma etching of HfO_2 gate-stacks is also computationally investigated with an emphasis on the selectivity between HfO_2 and Si.

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