Multi-scale Simulation Study for the Role of High C/F ratio Plasma on Etch Selectivity of SiO_2 and Si_3N_4 in q-ALE

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Using multi-scale simulation techniques, we studied how C/F ratio in plasma affected the etch selectivity between Si_3N_4 and SiO_2 with a formed thin FC film on each surface during a q-ALE process. In SAC etching for via or contact holes into oxide to make a contact, nitride also can be etched, resulting in the yield issue. Thus, we need to reduce the nitride loss effectively. However, as the device becomes smaller, it is hard to control to obtain enough selectivity. Previous experiments with various C_xF_y gases showed the enhancement of etch selectivity between Si_3N_4 and SiO_2 with high x/y ratio gas. However, the understanding of the underlying behavior has been not clear. First, we revealed the relationship between intrinsic C/F ratio neutral and species fluxes by using the plasma simulation, observing that high C/F ratio gas could create high C/F ratio radicals. With atomistic Molecular Dynamics (MD) simulation and DFT calculation, we also studied the possible role of C/F ratio on FC film formation on both substrates and following an ion bombardment. MD simulation results showed that with higher C/F ratio plasma, harder and denser FC film could be formed on Si_3N_4 by significantly increasing absorbed carbon (C), Si-C, and C-C bonds. In the SiO_2 case, we could observe many O-C bonds that cause to weaken the formed FC film by converting it to highly volatile materials (i.e., CO_2). The highest C/F ratio gas case showed that significant O-C bonds on SiO_2 were generated. Following the ion bombardment step with both modified substrates, we observed that the highest C/F ratio case exhibited less loss of total atoms and regenerated Si-C bonds, probably a dangling bond behavior. In Si_3N_4, N-C bonds were generated more to protect the substrate but not in SiO_2; O-C bonds were lost during the ion bombardment. We confirmed the surface reaction with DFT calculation. It showed that both Si and N removal was difficult without F, while O removal was possible even without F. Thus, we determined that Si_3N_4 etching was more F-limited than Ox, indicating that selectivity at high C/F ratio gas would be improved. Based on all findings, We concluded that using the plasma with high C/F ratio radical helped to increase selectivity by protecting Si_3N_4 more with denser and harder FC film but not on SiO_2 due to the O-C bonds in formed FC film. This study will help to understand the fundamental behavior of the dielectric selectivity with various C/F ratio plasmas during the q-ALE process and ultimately provide the guideline for the experiment.