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Effect of Hydrogen in the Plasma-Enhanced Atomic Layer Etching of Silicon Nitride: A Molecular Dynamics Study

Univ. of the Philippines[1], Osaka Univ.[2], Sony Semi. Corp.[3], °(M2)Jomar Tercero[1,2*], Akiko Hirata[3], Michiro Isobe[2], Masanaga Fukasawa[3], Magdaleno Vasquez, Jr.[1], and Satoshi Hamaguchi[2]

[*]E-mail: jutercero@ppl.eng.osaka-u.ac.jp

An understanding of the mechanisms of silicon nitride (Si_3N_4) atomic layer etching (ALE) [1,2] is crucial to help obtain atomic-level control in fabrication of microelectronic devices.[3] To help understand the process, we studied a plasma-enhanced ALE of Si_3N_4, using molecular dynamics (MD) simulations. Typically, this process consists of two alternating steps: the modification step, where the system is exposed to chemically reactive species that modify the surface layer, and the removal step, where low-energy ions are injected into the modified layer to sputter off the surface modified layer. The influence of hydrofluorocarbon (HFC) radicals used in the modification step was also studied by considering a hydrogen-rich (CH_2F) and a fluorine-rich (CHF_2) reactive species. In the simulation, it has been observed that hydrogen plays a crucial role in scavenging F atoms in the modified layer and eventually in reacting with nitrogen in the substrate layer, forming NH_x species. In addition, carbon atoms tend to remain in the surface after low-energy ion bombardment by forming a high-density SiC layer. The results were also compared with experimental observations and they were found to be in good agreement. The removal rates of both HFC and substrate layer were also estimated from the slopes of the depth change and found to depend strongly on the hydrogen content of the HFC used in the modification step.

References

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