Challenges for the development of plasma-based atomic layer processing – numerical and experimental analyses of plasma-exposed surface reactions at the atomic level

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As the sizes of semiconductor devices continue to diminish and are now approaching atomic scales, the downsizing of transistors following Moore's law is bound to end in the near future. The continuing market demand for higher performance and lower energy consumption of large-scale integrated (LSI) circuits therefore necessitates further innovation in semiconductor technologies. For example, new device technologies such as three-dimensional (3D) device structures and devices based on non-silicon materials have been invented to circumvent the requirement of further device miniaturization. The precise control of device structures at the atomic level over a large area is crucial for the manufacturing of such devices and atomic layer processes, i.e., atomic layer deposition (ALD) and atomic layer etching (ALE), are considered to be some of the most effective means to achieve such goals. Unlike conventional deposition or etching processes, an atomic layer process requires self-limiting reactions, i.e., surface reactions that limit the process only to (essentially) a monolayer in each process cycle and therefore allow a highly uniform process over a large area. The exact surface reaction mechanisms that allow the self-limiting processes, however, have not been well understood. In this work, we discuss our recent study on molecular dynamics (MD) simulations for plasma-based ALE processes for SiO_2 and SiN as well as beam-based experimental study on surface chemical reactions of low-energy incident reactive species with surfaces of Si-based materials and metals. Such analyses can give insight into the mechanisms of self-limiting surface reactions.