Modeling of plasma-enhanced ALD for silicon oxide films as clarification of fundamental deposition mechanism

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Plasma-enhanced atomic layer deposition (PEALD) has increasingly taken an important role in semiconductor manufacturing because of its ability to realize high step coverage deposition with low processing temperatures. Deposition of silicon oxide (SiOx) films is one of the most widely used applications of PEALD. Many research groups have studied PEALD-SiOx processes with aminosilane precursors and oxygen plasma; not only due to their industrial significance, but also for scientific interest. For example, such SiOx films can be deposited at temperatures as low as ambient; i.e., the relevant surface reactions can take place even at such low substrate temperatures. In this study, we aim to clarify the deposition mechanism in PEALD-SiOx by using both experimental and computational analysis, focusing now on the plasma oxidation step, since several previously published studies have already detailed the precursor adsorption steps. For example, those studies demonstrated differing saturation trends on growth per cycle with the type or number of amino ligands. In this study, we estimated both the generation of oxidation species and their surface reaction paths by performing quantum mechanical and numerical analyses. We then constructed a surface oxidation model including various aminosilane precursors that enabled the comparison of this analysis with experimental trends.