Thermal Decomposition Reaction Mechanism of Ultrathin Oxide on Si(111)

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The inhomogeneous decomposition of thin silicon oxide layers has been studied in some details recently to well understand the thermal stability of the ultrathin gate dielectric film (< 1 nm) employed in metal-oxide-semiconductor (MOS) devices [1, 2]. In the present study, the decomposition kinetics of ultrathin oxide on Si(111) have been investigated by real-time photoelectron spectroscopy using He-I resonance line (21.2 eV) and synchrotron radiation (710 eV) at BLSU23, SPring-8 [3] as functions of T and θoxide to clarify the void nucleation and 2D enlargement mechanism during oxide decomposition.

The wholly oxide covered Si(111) surface prepared by exposing O2 at 500 °C and P O2 = 4.6 × 10⁻⁵ Pa was decomposed by increasing T at the same time of stopping O2 supply as shown in Fig. 1. The decreasing feature of O 2p photoelectron intensity I O-2p likely shows a sigmoid-type function as demonstrated in Fig. 2. However, we need two kinds of fitting parameters at θoxide above and below ~0.3 ML (called regions 1 and 2, respectively) independent of T. This implies that the decomposition rate is significantly reduced at θoxide smaller than ~0.3 ML. In both regions 1 and 2, however, the activation energies are almost the same as 2.8-2.9 eV, suggesting that the rate-limiting reaction is SiO desorption. Furthermore the correlation between changes of work function and I O-2p was measured to consider the surface migrating species and the θoxide dependences of the oxidation state and oxidation-induced strain were monitored during the decomposition.