Initial Oxidation of Si(111)-7×7 Surfaces Studied by Photoelectron Spectroscopy Combined with Medium Energy Ion Scattering

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Abstract

Atomically clean Si(111)-7×7 surfaces were oxidized at room temperature (RT), 500 and 600℃ and the oxidized surfaces were analyzed *in situ* by synchrotron-radiation-light induced photoelectron spectroscopy and by medium energy ion scattering (MEIS). The absolute quantities of O and Si atoms forming oxide layers were determined precisely by MEIS as a function of oxygen exposure (*L*: Langmuir: 1×10^{-6} Torr・*s*). We also measured the Si *2p* core level spectra, from which the coverage of each oxidation state (Si^{+}, Si^{2+}, Si^{3+} and Si^{4+}) was determined. The present results showed that the oxidation at RT was almost saturated with O coverage of 1.7 ML (1 ML: 0.783×10^{15} atoms/cm^2) at O_2-exposure of 5 *L* under O_2 pressure of 1×10^{-8} Torr and the backbonds of the adatoms and rest atoms were almost oxidized. At this stage, the 7×7 pattern was still observed by reflection high energy electron diffraction. It is concluded that the atomic configuration dominating the oxidized surface is a 'ins-ins-ins-ad' structure (an O atom bonding on top of a Si adatom (rest atom) and three O atoms are inserted into three backbonds of adatom (rest atom)). The oxidation at 500℃(1×10^{-7} Torr) is almost saturated at O_2-exposure of 50 *L* with oxygen coverage of 2.9 ML and the oxide layer basically consists of two types of domains with intrabilayer and interbilayer termination. The oxidation at 600℃(1×10^{-5} Torr) is saturated with the O coverage of 4.1 ML and the oxide/Si(111) interface is also terminated with the above two types of structures.

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