Initial Oxidation of Si(001)-2×1 Surface Studied by Photoelectron Spectroscopy Coupled with Medium Energy Ion Scattering

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Abstract

Clean Si(001)-2×1 surface with a double-domain dimer structure was oxidized at room temperature (RT) under O_2 pressure of 1×10^{-8} Torr. The oxidation is almost saturated at O_2-exposure of 10 L (1 L: 10^{-6} $Torr \cdot s$) with O_2 coverage of 1.30±0.05 ML (1 ML: 6.78×10^{14} atoms/cm^2), which was measured by medium energy ion scattering (MEIS). There exist two oxidation stages, rapid (0 to 10 L) and very slow (≥ 10L) oxidation regimes. In the slow oxidation regime, the O-adsorption rate was estimated to be $0.5\text{-}1.0\times10^{-4}$ ML/L and the O atoms are adsorbed to on-top sites. The Si-2p core level analysis using synchrotron radiation-light revealed the fact that the high oxidation states Si^{3+} and Si^{4+} appear and have large fractions even at the early stage of the oxidation. As another information, the Si^{4+} state atoms tend to take the position of the top surface and other oxidation states atoms are distributed in the top and 2nd layers. The present results indicate that the initial oxidation does not proceed in a laterally uniform fashion but occurs as the formation of microscopic oxide complexes distributed randomly. Considering the absolute O coverage and the fractions of oxidation states, we propose a possible structure model for the initial oxidation of the Si(001)-2×1 surface at RT.

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