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STM Analysis of Site Selectivity in the Initial Oxidation of Si

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The pressure and temperature-dependent site selectivity of oxygen in the initial oxidation of the Si(111)-7x7 surface was investigated using a scanning tunneling microscope. At room temperature, two different oxygen-induced features, bright and dark sites, were observed indicating two different oxygen chemisorption configurations. As the oxygen dose increased, the number of dark sites increased whereas that of bright sites did not seem to change noticeably. Both the bright and dark features preferred the adatom sites of the faulted half to those of unfaulted half of the DAS structure. In particular, the bright features preferred the corner adatom sites to center ones while the major dark sites preferred the center adatom sites. The site preference of the dark features to center adatom sites has not been reported yet and can be attributed to the slow oxygen exposure(1×10^{-9} torr) which gives oxygen atoms sufficient diffusion time to be adsorbed on the most stable sites, center adatom sites. This site-dependent oxidation of Si under low O_2 pressure disappeared at the same O_2 exposure under higher O_2 pressure(5×10^{-8} torr) due to the lateral interaction of adsorbed oxygen species resulting in the decrease of the surface diffusion of adsorbed species. When oxygen was exposed at 550 °C, no bright site was observed indicating that the bright site is thermally unstable. The dark features still preferred the adsorption at faulted sites and the center ones. This result obtained at high temperature suggests that oxygens with high kinetic energy are distributed in two different adsorption sites giving a preference to center sites.