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XPS and SHG Analysis of Initial Oxidation of Si(111) with Ozone

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Abstract

Initial oxidation of Si(111) surface with ozone was investigated by X-ray photoelectron spectroscopy (XPS) and second harmonic generation (SHG). High purity ozone jet (ozone concentration; over 80% at the sample surface) which was generated by the evaporation of liquid ozone was used for the initial oxidation of the surface showing 7x7 LEED pattern. Both the intensities of O-1s XPS peak and second harmonics (SH; 532 nm) generated for the incidence of Nd:YAG laser (1.064 μm) were measured as a function ozone exposure (Langmuir unit). For comparison, the XPS and SHG intensities were also measured for oxygen (i.e., molecular oxygen) exposure.

The SHG intensity decreased very rapidly for initial exposure (less than a few Langmuir) of ozone/oxygen, and then came to steady states for further exposure. The decay rate of the SH intensity in the initial exposure region was nearly the same for ozone and oxygen, but the steady state intensity was different. On the contrary, O-1s peak intensity increased very rapidly for initial exposure of ozone/oxygen, and then saturated. The increasing rate in the initial exposure region was larger for ozone than oxygen, and the saturation intensity was also higher for ozone. These results can be considered as follows: Ozone molecules dissociates at the sample surface and yields oxygen molecules and atomic oxygen. The former adsorbs on the sample surface as in the case of oxygen exposure, terminating dangling bonds of Si resulting in the decrease of SH intensity. The atomic oxygen does not adsorb on the dangling bonds, but inserts into backbonds of Si. Since the escape depth of O-1s electron is about 2 nm, oxygen insertion to the backbonds is detectable by XPS. However, it could not be detected by SHG probably because it is not so sensitive to SHG as dangling bond termination.

Different oxidation mechanism by ozone (mainly due to the contribution of atomic oxygen) was clearly shown for the oxidation of hydrogen terminated Si(111) surface. It was confirmed that ozone can oxidize the Si surface terminated with hydrogen at monohydride condition in spite that oxygen molecules can hardly react with the surface.

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