

Abstract No. ghos0214

Structural Changes of Si(111)7x7 During Successive Stages of Oxidation

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Beamline(s): X16A

The surface x-ray diffraction technique has been used to measure the inplane superlattice reflections from the clean as well as oxygen dosed Si(111)7x7 surface using the X16A beamline at National Synchrotron Light Source, Brookhaven. About fifty structure factor intensities are enough to determine atomic structure in 2D of Si(111)7x7 structure, assuming p6mm symmetry. We have observed the O₂ interaction with Si(111)7x7 as a function of dose at room temperature. At the initial stage (< 1 L, $1L = 1 \times 10^{-6}$ Torr. Sec) the measurements as shown in the figures show a trend in the structure factors. The 7,3 and 3, 0 structure factors have large contributions from adatoms. These structure factors increase initially then decrease, suggesting two stages of oxidation. Two stages of oxidation were also seen in STM measurements for 1L and ~ 8 L structures. Difference Fourier maps as shown in the figure for the lower dose case gives real space mapping of the changes due to the oxidation processes and corresponding structural changes of Si(111) 7x7 surface. The triangular section is an asymmetric section for the 7x7 unit cell with adatoms (large circles) and other atoms (small circles) for an ideal 2D 7x7 surface model. Until now, we have not found a simple fitting model of a modification to the atomic structure to account for the successive stages of oxidation. Results from these models would answer some of the unresolved questions regarding the oxidation of Si(111)7x7 surfaces.

This work is supported by Air Force Office of Scientific Research MURI grant, # F49620-01-1-0336.

