Structural analysis of ethylene chemisorbed Si(001) surface studied by photoelectron diffraction

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Introduction

Ethylene is the simplest hydrocarbon molecule with π bonding orbital, and clarifying the reaction of the molecule with dangling bonds on Si(001) 2x1 surface is to be a fundamental information for all molecules with unsaturated bonds on Si substrate. Many of theoretical and experimental researches [1-4] have been performed so far to clarify the adsorption structure of ethylene, and a structure in which ethylene adsorb molecularly with remaining Si dimers has been accepted. Recently, drastic decrease in adsorption rate of ethylene over the coverage of half a monolayer (ML, density of C atom to Si atom) has been pointed out by a study using high-resolution photoelectron spectroscopy [4].

In this study, we have performed structural analysis for the surface covered with ~0.5 ML of ethylene by photoelectron diffraction (PED).

Experiment and simulation

The PED experiment has been carried out on an undulator beamline, BL-13C. An UHV chamber attached to the beamline was equipped with a high-resolution analyzer (VG, CLAM4) and a motor controlled manipulator. The PED measurement was performed in azimuthal angle (denoted as ϕ here) scan mode for each polar angle (θ) with a fixed photon energy of 391 eV.

A Si(001) substrate with a minute miscut-angle was used for PED measurement. Before the PED measurements, Si substrates were flashed and annealed, resulting in forming the single-domain (SD) 2x1 structure. The domain ratio (major domain coverage) of the surface was checked by LEED spot intensity and it was ~9 : 1. The Si(001) 2x1 surface was exposed to 10 Langmuir of ethylene gas at room temperature through a variable leaking-valve for both experiments. The adsorption rate changes drastically about that dosage.

For the simulation, we have used a multiple scattering simulation program, MSCD, based on Rehr-Albers formalism [5]. We have assumed a cluster radius of 12 Å, which includes over 200 atoms.

Results and discussion

Figure 1 shows the experimental and simulated PED patterns of C 1s core-level for the ethylene-adsorbed surface along with schematic of models used in the simulation. The simulation curves of model A, which corresponds to a single molecule adsorption, are in good agreement with those of experiment. On the other hand, the simulation curves of model B, in which the other ethylene molecules surround the emitter, have unnecessary peaks at ϕ=40-70°. R-factor values of model A and B are 0.13 and 0.22, respectively. This result indicates that ethylene hardly chemisorbs to the neighboring site of a chemisorbed site in a dimer row at this dosage. Based on the effective distance of PED from an emitter for low-energy photoelectron, model A corresponds to p(2x2) and c(4x2) structures whose coverage is 0.5 ML.

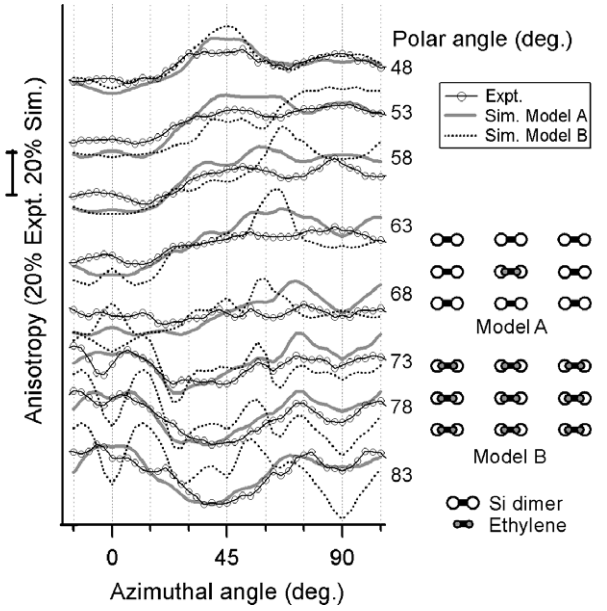

Fig. 1 C1s PED patterns of ethylene adsorbed Si(001) surface. Circles with thin line, thick gray line, and dotted line correspond to experiment, simulation with model A, and that with model B, respectively. Schematic of the models is also inserted.

The effect of structural distortion caused by repulsion between hydrogen atoms of neighboring ethylene species [3] is considered to the model A and it was found that this effect does not improve the simulation pattern.

References

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