

Structural analysis of thiophene chemisorbed Si(001)-(2x1) surface

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Introduction

Thiophene that contains a sulfur atom in the five-membered ring is an attractive molecule technologically, because it is the building block of polythiophene that can be a conductive polymer. Numerous researches of adsorption of thiophene on metal surfaces have been performed in the catalytic field, however limited studies were carried out on semiconductor surfaces. On Si(001)-(2x1) surface, the formation of 2,5-dihydrothiophene like species has been found by the valence band and high resolution electron energy loss spectroscopy (HREELS) studies [1,2].

In this study, we have performed structural analysis for the thiophene chemisorbed Si(001)-(2x1) surface by photoelectron spectroscopy (PES).

Experimental

The PES 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).

A Si(001) substrate with a minute miscut-angle was used to avoid step-derived extrinsic adsorptions or dissociations. Before the PES measurements, Si substrates were flashed and annealed for cleaning in UHV. Then, clear (2x1) LEED spots were observed. After cooling down the sample to room temperature, the surface was exposed to thiophene gas until the saturation coverage. The thiophene-saturated surface still showed (2x1) LEED spots with conserving the Si dimer structure.

Results and discussion

Figure 1a shows a typical S 2p PES spectrum of the thiophene-adsorbed surface with the curve fitting result. Two components separated by ~1.0 eV (S1 and S2) are needed to fit the spectrum. Either component could be assigned to sulfur in the 2,5-dihydrothiophene like species that is expected by HREELS study [2]. However, at least one more species must exist even just after the adsorption. An adsorption species of a molecule such as thiophene may be transformed the structure to more stable one or decomposed by a photo-excitation. We have quantified the percentage of the components as a function of the irradiation time of SR-beam at 270 eV (Fig. 1b). The component S1 (S2) decreases (increases) as the irradiation time increases. No other component was found after the irradiation for over 3 h.

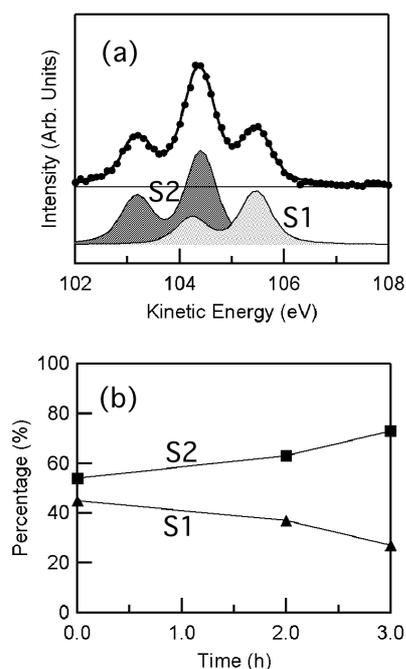


Fig. 1. (a) The typical S 2p PES spectrum of thiophene-adsorbed Si(001)-(2x1) surface taken at photon energy of 270 eV with the curve fitting result. (b) The percentage of the component S1 and S2 as a function of irradiation of the SR beam ($h\nu = 270\text{eV}$).

We have also measured the Si 2p spectra of the thiophene-adsorbed surface. After the adsorption, components derived from the asymmetric Si dimer structure completely disappear, and instead of these, two surface components appear at the binding energy of +0.28 and +0.90 eV from the bulk component. In latter case, the energy shift is relatively large. Hence a Si atom, bonded to a S atom whose electro-negativity is rather high, may exist. Time dependence of these components during light irradiation same as Fig. 1b, which has not been measured yet, would make clear the ambiguity of the stable and meta-stable adsorption structures.

References

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