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Chemical reactivity of asymmetric dimer on Si(100)(2x1) by means of high resolution Si 2p photoelectron spectroscopy

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Introduction

There are many reports about the adsorption of inorganic and organic molecules on the Si(100)(2x1) surface [1-3]. Recently we have proposed a general reaction mechanism for chemisorption on Si(100)(2x1), where the asymmetric dimer of Si(100)(2x1) should play an important role for the reaction: the up atom of the dimer (S_u) acts as Lewis base and the down atom at the same dimer (S_d) acts as Lewis acid. Thus, we expect that Lewis-base molecules preferentially react with the S_d and on the other hand Lewis-acid molecules react with S_u. High resolution Si 2p photoelectron spectroscopy (HR-PES) is one of the ideal methods to elucidate the nature of the interface bonding between molecules and the Si(100)(2x1) surface, because we can discriminate the Si atoms at different chemical environment using surface core-level shift [5, 6].

Experimental

The experiments were performed with an undulator source of the beam line BL-16B at Photon Factory in Tsukuba, Japan. The base pressure of the chamber was below 1×10^{-10} Torr. All of the Si 2p spectra shown in this paper were obtained using a hemispherical electron analyzer. The total instrumental energy resolution was < 80 meV.

A p-type (B-doped, 3~5 Ωcm) Si(100) wafer was cleaned by being outgassed at ~900 K for 12 hours, flashed up to ~1500 K several times, and cooled slowly from ~1000 K to ~100 K. After this treatment, the sharp Si(100)c(4x2) LEED pattern was observed. Gaseous molecules were introduced onto the surface by means of a pulse gas dosing. As Lewis-base molecules, NH_3, CO, pyridine etc., and as Lewis-acid BF_3 and CO_2 were adsorbed on Si(100)(2x1).

Results and discussion

A. clean Si(100)c(4x2) surface

Figure 1 shows Si 2p PES spectra ($h\upsilon$=129 eV) for the clean Si(100)c(4x2) surface at 60° emission angle, where B: bulk, S_u: up dimer, S_d: down dimer, SS: second layer, X: unknown component [7]. The fitting curve is solid line and the experimental data are open circles. These are in good agreement with the previous report by Landemark et al [6].

B. CO adsorbed Si(100)c(4x2) surface

The initial stage of CO adsorption on Si(100)c(4x2) has been carefully investigated by means of Si 2p HR-PES. Imamura et al. [7] have reported that CO adsorbs on Si(100)(2x1) via σ-donation mechanism, i.e., CO acts as Lewis-base. Thus we have expected that CO reacts with S_d preferentially at low coverage. By our careful analysis of the present experimental data, the S_d component is initially decreased in intensity but the S_u component does not change at low coverage, and an additional peak newly appears at –0.05 eV which is assigend to the surface Si atoms reacted with CO.

Other adsorption systems were also investigated by using Si 2p and valence PES, and the data is now being analyzed.

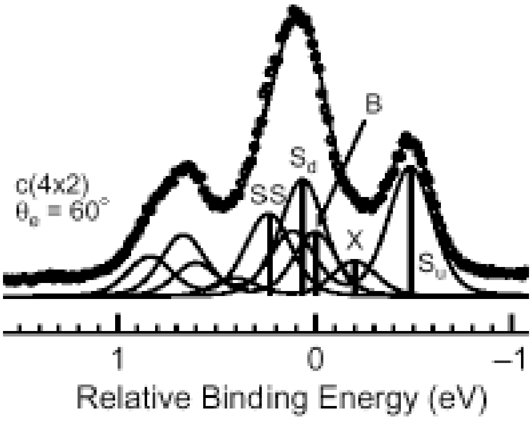

Figure 1 Si 2p HR-PES of clean Si(100)c(4x2)

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